Periodic Table of the Elements

IUPAC Notation

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

Previous IUPAC Notation

IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA	IB	IIB	IIIB	IVB	VB	VIB	VIIB	0

1 H 1.01																	2 He 4.00
3 Li 6.94	4 Be 9.01											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98.91)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57–71 See Lantha-nides	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209.98)	85 At (209.99)	86 Rn (222.02)
87 Fr (223.02)	88 Ra (226.03)	89–103 See Acti-nides	104 Unq (261.11)	105 Unp (262.11)	106 Unh (263.12)	107 Uns (262.12)	108 Uno	109 Une	110 Uun								

57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (144.91)	62 Sm 150.36	63 Eu 151.97	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
89 Ac 227.03	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu (239.05)	95 Am (241.06)	96 Cm (244.06)	97 Bk (249.08)	98 Cf (252.08)	99 Es (252.08)	100 Fm (257.10)	101 Md (256.09)	102 No (259.10)	103 Lr (262.11)

Lanthanides

Actinides

Dictionary of Inorganic Compounds

VOLUME ONE

Ac–C_{10}

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VOLUME ONE

Ac–C_{10}

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Supplements to *Dictionary of Inorganic Compounds* will be published each year subsequent to publication of the Main Work. The first annual supplement will be published in Autumn 1993.

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The Editor is always pleased to receive comments on the selection policy of the Dictionary, and in particular welcomes specific suggestions for compounds or groups of compounds to be considered for inclusion in the annual supplements.

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Preface

Inorganic compounds play a vitally important role as industrial feedstocks, fine chemicals and advanced materials, and in life processes. Their most outstanding feature is perhaps their great structural diversity. Whilst this diversity makes inorganic chemistry a rich and exciting branch of science, it also makes its documentation in a unified and consistent manner particularly challenging. The *Dictionary of Inorganic Compounds* has been designed to meet this challenge by presenting the essential information on the most important inorganic substances in a well organised manner. The Dictionary appears at a time when inorganic chemistry is enjoying a resurgence of interest, although as scientific research becomes more interdisciplinary, it may be undertaken within various departments.

The idea of a companion inorganic dictionary to the well known *Dictionary of Organic Compounds* is an obvious one, but the technical and editorial problems which have had to be overcome, in view of the greater structural and organisational diversity of the data, have been considerable. Thus the resulting dictionary represents the results of an intensive effort by a large team over some five years, as well as a great deal of technical development work by the Publishers.

The definition of inorganic chemistry used in this Dictionary is a wide one and encompasses not only molecular, coordination and non-molecular compounds, but also special materials such as bio-inorganics, superconductors, ceramics and minerals. The 22,000 entries included are those felt by the editorial team to be most representative of the elements concerned and those of interest to a wide range of scientists for their applications or potential applications. It is expected that the Dictionary will fulfil the role of an essential point of first access to the literature and that it should encourage browsing by the specialist and non-specialist alike. Annual supplements are planned to enhance the usefulness of the whole publication and to retain its topicality.

Some omissions and inaccuracies are inevitable in an undertaking of this size and we would appreciate their being pointed out to the Publisher so that they can be rectified.

B.J. Aylett
P. Day
E.A.V. Ebsworth
W.P. Griffith
N.N. Greenwood
R. Thompson

Introduction

1. Using the Dictionary

The arrangement of entries is in order of empirical formula according to the Hill Convention (i.e. C, then H, then other elements in alphabetical sequence of element symbol). Where no carbon is present, the elements including H are ordered strictly alphabetically.

Every entry is numbered to assist ready location. The entry number consists of the prefix IC for Inorganic Compound followed by a six-digit number. In these main work volumes the first digit is always 0; entries in the supplements will have the supplement number as the first digit.

Volume 4 contains three indexes. The index of commonly occurring structural types lists non-molecular compounds of selected lattice types such as NaCl-type, CsCl-type, rutile-type, perovskite-type. The name index lists every compound name and synonym in alphabetical order. The CAS Registry Number Index lists all CAS numbers included in the Dictionary in serial order.

The fifth volume contains the element index which is divided into sections according to each element of the period table. Each section is ordered alphabetically by element symbol. Within each section are listed all compounds containing that element, in formula order. Thus sodium sulfate (Na_2SO_4) appears in three of the element index sections under sodium, sulfur and oxygen.

All indexes refer to the entry number. Each index is described in more detail at its beginning.

2. Compound selection policy

In compiling this Dictionary the aim has been to include:

(*i*) The elements

(*ii*) Binary and ternary compounds including hydrides, halides, oxides, sulfides, selenides, tellurides, nitrides, phosphides etc.

(*iii*) Important coordination compounds

(*iv*) Compounds with an established use such as catalysts, starting materials, synthetic reagents etc.

(*v*) Other compounds of particular chemical, physical, biological, structural or historical interest.

Some groups of compounds were originally included in previous Chapman & Hall chemical dictionaries, particularly the *Dictionary of Organometallic Compounds*. Of the two main groups, the metal carbonyl complexes will continue to feature in both Dictionaries. However, the cluster boranes and metallaboranes will in future be confined to the *Dictionary of Inorganic Compounds* even though they may contain metal–carbon bonds.

3. Organisation of entries

Some compounds which are not considered sufficiently important to justify entries of their own have been included as variants or derivatives in main entries. Derivatives typically include hydrates, solvates, donor-acceptor complexes (adducts generally) or one of the following special categories:

3.1 *Isotopically labelled compounds*

The Dictionary includes data on only the most important isotopic variants, generally limited to those of hydrogen. Deuterium (^2H) and tritium (^3H) are denoted separately in formulae as atoms D and T respectively and are alphabetically indexed as for other atoms. Data for deuterium oxide (D_2O), for example, will be found within the entry for water.

Information on the most important isotopes for each element is provided within the entry for that element.

3.2 *Dimeric and oligomeric substances*

Where a compound is known in several states of aggregation, these are all included in a single entry which usually refers to the monomer. The empirical formulae of all the oligomeric forms are given as well as all appropriate synonyms, and the compound can therefore readily be traced through indexes, whether looked for as the monomer or the oligomer.

Compounds which are known only in dimeric form under normal conditions are entered as such but the hypothetical monomers are included as derivatives to ensure that the names and formulae of the monomeric forms occur in the indexes.

3.3 *Anions and cations*

Entries for ionic substances containing complex ions generally refer to the naked complex cation or anion and the formula, formula weight and CAS Registry Number given for the entry are those of the ion, in agreement with current CAS practice. Salts of the ion with various counterions are then treated as derivatives and the empirical formulae of the more important ones are given.

If a specific salt is considered to be of particular importance it will be given an entry of its own, but there will be a cross-reference between the entry for the complex ion and the salt.

3.4 *Minerals*

Wherever possible, minerals corresponding to synthetic compounds are included within the entry for the synthetic compound, e.g. Zinc blende and Wurtzite are incorporated into the entry for Zinc sulfide (ZnS). Only when the mineral is the sole point of interest or unavailable synthetically is it given an entry in its own right.

4. Literature coverage

In compiling these volumes the primary literature has been surveyed to the beginning of 1991 and some important later citations have been incorporated.

The first annual supplement will appear in mid-1993 and will cover the literature to mid-1992.

5. Organisation of data within entries

Fig. 1 illustrates the format of a typical entry. The range of information included within the entries is described in detail below.

5.1 *Chemical names and synonyms*

The naming of inorganic compounds can be exceptionally difficult. In selecting the range of alternative names to present for each compound or derivative, we have been guided by the following principles:

(*i*) The function of the Dictionary is to report names which are found in the literature, including Chemical Abstracts, and not to attempt to impose a system of nomenclature. Therefore the editorial generation of new names has been kept to the minimum required by consistency. The majority of names given in the Dictionary are those given in the original paper(s) and in Chemical Abstracts.

(*ii*) For compounds of complex structure, especially metal cluster derivatives where nomenclature is still evolving, only the Chemical Abstracts name is reported. Frequently, the authors of papers reporting such compounds do not attempt to name them and most users of the Dictionary wishing to locate such compounds will probably do so via the empirical formulae.

(*iii*) There are many examples in the primary literature of the naming of inorganic compounds which is definitely incorrect according to IUPAC convention, especially in the non-alphabetical ordering of ligands in coordination compounds. Many of these incorrect forms are reported here.

(*iv*) Trivial variations in nomenclature which do not materially affect the alphabetical ordering of the name are not included. Such minor variations are legion, e.g.:

(α,β,γ,δ-Tetraphenylporphyrinato)
(5,10,15,20-Tetraphenylporphyrinato)

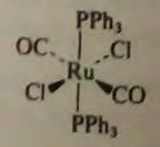
(*v*) The spellings used for the elements Al, Cs and S in this Dictionary are aluminium, caesium and sulfur respectively as recommended by IUPAC. (This is in contrast to the earlier *Dictionary of Organometallic Compounds* which used aluminum and cesium).

(*vi*) *Chemical Abstracts Service names*. Names corresponding to those used by CAS during the 8th, 9th, 10th and 11th collective index periods (1967–71, 1972–76, 1977–81, 1982–86 respectively) are labelled with the suffixes 8CI, 9CI, 10CI, and 11CI respectively. Names encountered in CA since 1986 are labelled 12CI although it is possible that some further changes may have occurred before publication of the twelfth collective index.

For the majority of inorganic compounds, the nomenclature brought in for the 9th Collective Index Period (and referred to as 9CI nomenclature) has since been unchanged. This is not true for some groups of compounds such as cluster boranes, where the nomenclature is still evolving. There are also many examples of the same compound being registered more than once under different names (and registry numbers) in CA.

The following suffixes which are to be found attached to CA names have been omitted:

(*a*) Stereochemical descriptors, for example, in Dicarbonyldichlorobis(triphenylphosphine)-ruthenium the CAS descriptor (OC-6-12) indicates the geometry shown below:



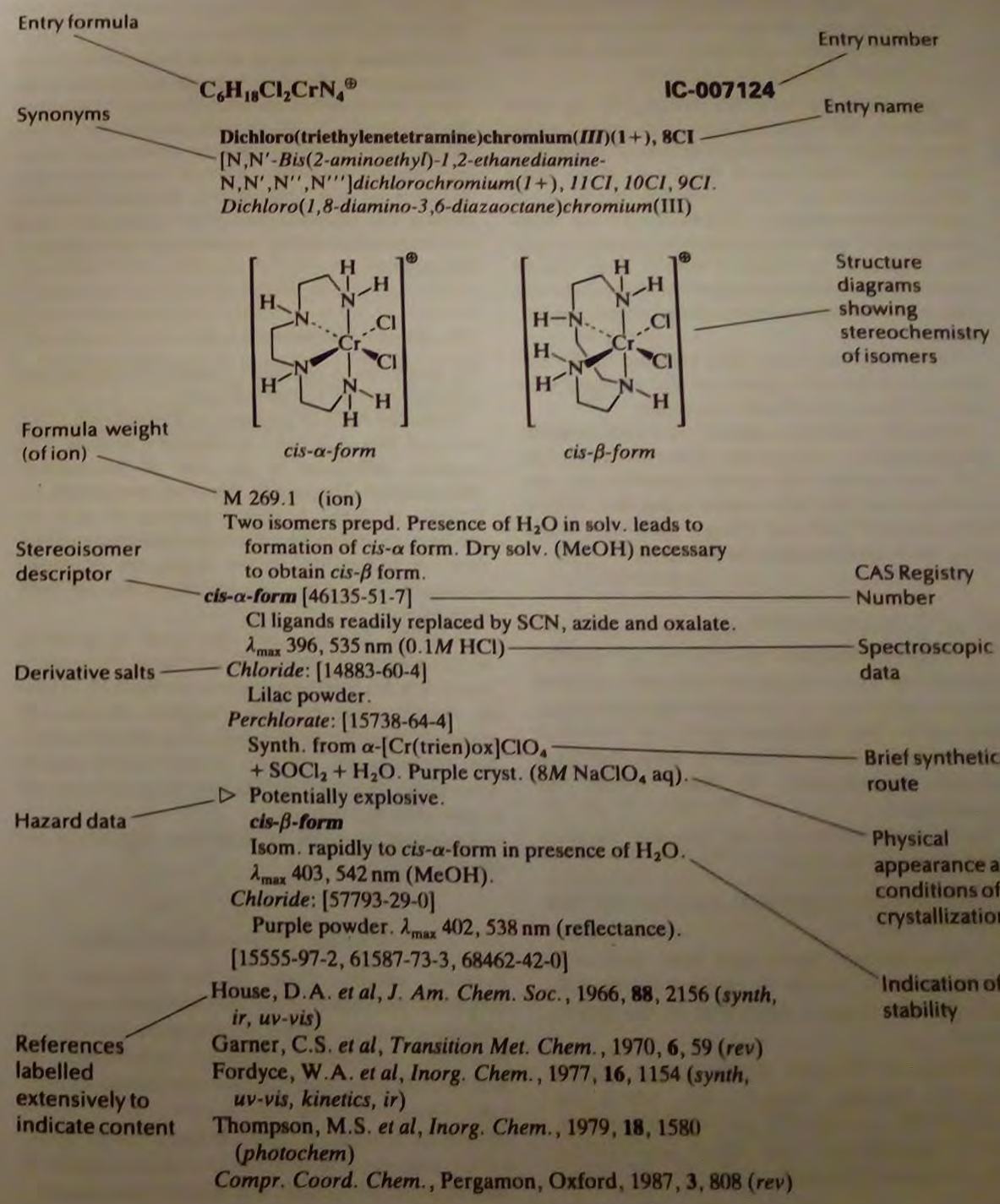

Entry formula
C6H18Cl2CrN4⊕
Entry number
IC-007124
Synonyms
Dichloro(triethylenetetramine)chromium(III)(1+), 8CI
Entry name
[N,N′-Bis(2-aminoethyl)-1,2-ethanediamine-N,N′,N″,N‴]dichlorochromium(1+), 11CI, 10CI, 9CI.
Dichloro(1,8-diamino-3,6-diazaoctane)chromium(III)
Structure diagrams showing stereochemistry of isomers
cis-α-form
cis-β-form
Formula weight (of ion)
M 269.1 (ion)
Two isomers prepd. Presence of H2O in solv. leads to formation of cis-α form. Dry solv. (MeOH) necessary to obtain cis-β form.
Stereoisomer descriptor
cis-α-form [46135-51-7]
CAS Registry Number
Cl ligands readily replaced by SCN, azide and oxalate.
λmax 396, 535 nm (0.1M HCl)
Spectroscopic data
Derivative salts
Chloride: [14883-60-4]
Lilac powder.
Perchlorate: [15738-64-4]
Synth. from α-[Cr(trien)ox]ClO4 + SOCl2 + H2O. Purple cryst. (8M NaClO4 aq).
Brief synthetic route
Potentially explosive.
Hazard data
cis-β-form
Isom. rapidly to cis-α-form in presence of H2O.
λmax 403, 542 nm (MeOH).
Physical appearance and conditions of crystallization
Chloride: [57793-29-0]
Purple powder. λmax 402, 538 nm (reflectance).
[15555-97-2, 61587-73-3, 68462-42-0]
Indication of stability
References labelled extensively to indicate content
House, D.A. et al, J. Am. Chem. Soc., 1966, 88, 2156 (synth, ir, uv-vis)
Garner, C.S. et al, Transition Met. Chem., 1970, 6, 59 (rev)
Fordyce, W.A. et al, Inorg. Chem., 1977, 16, 1154 (synth, uv-vis, kinetics, ir)
Thompson, M.S. et al, Inorg. Chem., 1979, 18, 1580 (photochem)
Compr. Coord. Chem., Pergamon, Oxford, 1987, 3, 808 (rev)

Fig. 1. A typical Dictionary entry

(*b*) Descriptors indicating metal-metal bonding, e.g. Hexa-μ-chlorohexachlorotriruthenate(4–) (*2Ru–Ru*). On the other hand, oxidation state has in many cases been inserted into CAS names, See Section (vii) below.

(*vii*) *Oxidation states and charges*. For any given substance, the oxidation state (also known as the Stock number) of the element of interest is incorporated into at least one of the names given, using Roman numerals or zero, provided that it can be unequivocally assigned. Oxidation states are therefore generally omitted from nitrosyl complexes where the assignment of oxidation state is often controversial, and also from compounds of elements having only one common oxidation state, where it is unnecessary.

The overall ionic charge (also known as the Ewens-Bassett number) of a complex is also provided in at least one name, using Arabic numerals.

Chemical Abstracts names do not describe oxidation states, only charges. However, where the CAS name is the only readily accessible one, the oxidation state has been added editorially. Where both oxidation state and charge occur in a single name, the former precedes the latter.

5.2 *CAS Registry Numbers*

CAS Registry Numbers are identifying numbers allocated to each distinctly definable chemical substance indexed by the Chemical Abstracts Service since 1957. The Numbers have no chemical significance but they provide a label for each substance independent of any system of nomenclature.

The following features of CAS Registry Numbers should, however, be noted:

(*i*) Hydrates, salts, complexes, etc. have their own registry numbers.

(*ii*) Stereoisomeric forms also have their own Registry Numbers, usually in addition to the non-specific Registry Number applicable to the generic substance.

(*iii*) Additional Registry Numbers may also be allocated to bonding isomers, etc., which are discussed in the literature but which have not been separately characterised (and which may not be capable of separate existence).

In this publication whilst every attempt has been made to achieve accuracy of the reported Registry Numbers, no guarantee can be provided as to the comprehensiveness of the range of numbers presented. Thus:

(*i*) The absence of a Registry Number for a particular substance does not necessarily imply that one has not been allocated.

(*ii*) Where the substance has been indexed more than once by CAS, one of the numbers (usually the lowest unless special considerations apply) is quoted for the main entry. All the others are listed at the foot of the entry in small typeface showing that other numbers are associated with the compound. Also included at this location are Registry Numbers dealing with stereoisomeric forms or hydrates which are not readily assigned to a more specific location in the entry.

5.3 *Empirical formulae*

As described in Section 1, empirical formulae are presented in Hill convention order.

Since the book is arranged in formula order, it is essential that each entry is assigned a formula. This presents difficulties in the case of incompletely characterised compounds. For such compounds the formula is shown in square brackets to alert the reader to its artificiality. Examples include complexes such as technetium citrate which are important commercially but whose composition has not been determined.

Artificial formulae are also used in grouping together series of closely related binary compounds where it is felt their organisation as a family is helpful to readers. For example, tungsten silicides are grouped together in this way. The specific names and formulae for different stoichiometries are all separately presented within the entry and may be accessed via the indexes.

Empirical formulae of important derivatives are provided.

5.4 *Formula weights (Relative Formula Mass)*

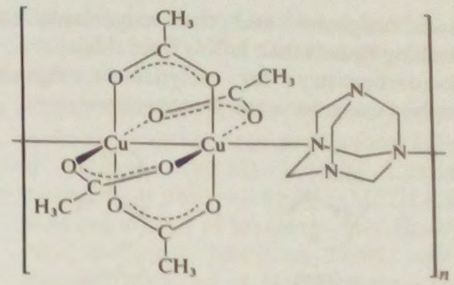
Formula weights given in the Dictionary are computer calculated from the formulae using the values for atomic weights published by the IUPAC Inorganic Chemistry Division, Commission on Atomic Weights and Isotopic Abundances; *Pure Appl. Chem.*, 1991, **63**, 975.

Formula weights are given to one decimal place, but is it important to note that *the atomic weights of some elements are variable within wider limits than this implies*. This applies not only to radioactive or radiogenic elements such as U and Pb but also to some non-radioactive elements, especially Li and B which exhibit a wider variation in commercially available samples.

5.5 *Structural representations*

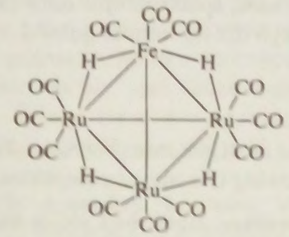
In preparing this Dictionary, care has been taken to achieve as much consistency and clarity in the presentation of structural formulae as possible. The primary aim has been to indicate the connectivity and, where known, the stereochemistry.

The diagrams are necessarily stylized and are intended to convey the correct topochemistry rather than to convey accurate representations of bond lengths and angles.

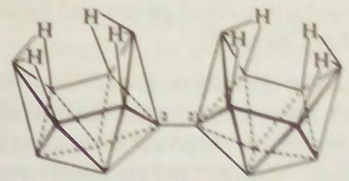


Bonding. The bonding in many transition metal complexes and clusters is more or less complex and subject to varying interpretation, and is therefore not amenable to accurate depiction by the conventions which serve reasonably well for organic compounds.

Bridging hydrogens between two metal centres are depicted for clarity as though there are full metal–metal bonds though there is rarely so much electron density between the two metals, e.g.:



Boranes. BH groups in the cluster boranes and related species are represented by vertices, as shown below:



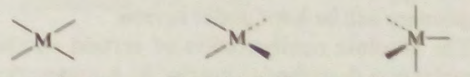
Only when B is bonded to 2 (or more) non-bridging atoms is it depicted explicitly. All other atoms, including carbon, are depicted explicitly.

This convention is analogous to the representation of CH_2 or CH groups as plain vertices in organic compounds and which is also used to depict ligands in this dictionary.

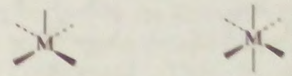
Polymeric transition metal complexes. Wherever possible the coordination polyhedron of the metal is depicted, and the points of attachment to the next unit are indicated using bonds that extend outside square brackets, e.g.

5.6 *Stereochemical conventions*

The various coordination polyhedra are depicted using wedged and dashed bonds, the most common polyhedra being:



Square planar — Tetrahedral — Trigonal bipyramidal



Square pyramidal — Octahedral

The shapes of polyhedra greater than 6 are not amenable to clear representation by this means and a textual statement such as 'square antiprismatic' is combined with the diagram.

The terms 'tetrahedral' and 'octahedral' are used in a general sense and do not imply strict symmetry types. For the latter, the point group descriptors T_d and O_h are employed.

Octahedral complexes. In the case of complexes bearing two different types of substituent the stereochemistry is adequately defined using the terms *cis*, *trans*, *fac* or *mer*:

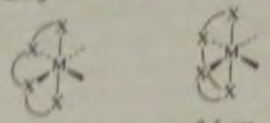
cis — *trans* — *fac* — *mer*

In more complicated cases, italicised letters are used to designate the positions of ligands in various configurations. The letters are assigned thus:

The first mentioned alphabetical ligand in the name is given the designator *a*, the second ligand the next

lowest designator and the assignments to the remaining ligands then follow from this.

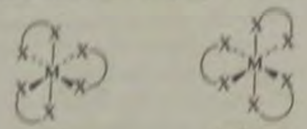
Stereochemistry for polydentate ligands is described using the α and β convention:



α-form *β-form*

During the compilation of this Dictionary, IUPAC adopted the *Configuration Index* notation based on Cahn-Ingold-Prelog (CIP) rules which is also to be found in Chemical Abstracts. An example is given in 5.1 (vi). Possible incorporation of such descriptors into supplements and future editions of this Dictionary will be kept under review.

The absolute configuration of certain octahedral complexes is described using the Δ, Λ convention,



Λ-form *Δ-form*

5.7 *Importance/use*

Information on the use of an inorganic compound is given when it has an established laboratory or industrial use or where it has been shown to undergo or catalyse reactions of potential usefulness.

5.8 *Physical data*

(*i*) **Interatomic dimensions.** Selected dimensions, usually obtained by x-ray crystallography, are provided: bond lengths are given in picometres ($pm = 10^{-12}m = 10^{-2}Å$), and angles in degrees.

(*ii*) **Melting points.** Melting points are recorded in degrees Celsius (°C). The policy followed in the case of conflicting data is as follows:

(*a*) Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted.

(*b*) Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure) the lower figure is given in parentheses, thus: Mp 139° (132–133°).

(*c*) Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted, thus: Mp 142°, Mp 205–206°.

(*d*) Known cases of polymorphism or double melting point are noted.

(*iii*) **Boiling points.** These are recorded in degrees Celsius at ambient pressure unless indicated by a subscript representing the pressure in mmHg of the measurement, e.g. Bp_{20} 130°.

(*iv*) **Sublimation temperatures.** These are recorded in a similar style to boiling points, e.g. $Subl_{20}$ 130°.

(*v*) **Thermodynamic data.** Limited thermodynamic data are provided; in other cases these can be located through the references quoted.

(*vi*) **Spectroscopic data.** Spectroscopic data such as ir maxima and uv wavelengths and extinction coefficients are given in many cases where spectroscopic identification has been important in characteristisation, particularly for unstable compounds. In many other cases, spectroscopic data can be rapidly located through the references quoted.

5.9 *Units*

Units have, in most instances been standardised to SI, with the following two major exceptions.

(*i*) **Temperature.** Both the Celsius and the Kelvin scales are used, depending on the quantity being measured. Temperatures at which magnetic data have been recorded (typically magnetic moments) and low temperatures generally are quoted in Kelvin (K) following observed practice. All other temperatures, particularly melting points and boiling points, are quoted in Celsius (°).

(*ii*) **Pressure.** Pressures lower than 1 standard atmosphere are quoted in millimetres of mercury (mmHg, which is equivalent to torr). Higher pressures are quoted in standard atmospheres (1 atm. = 1.01325 bar = 101325 Pa).

5.10 *Toxicity and Hazard Information*

(*i*) **General.** Toxicity and hazard information is highlighted by the sign ▷ (which also appears in the indexes.

The field of safety testing is a complex, difficult and rapidly expanding one, and while as much care as possible has been taken to ensure the accuracy of reported data, the dictionary must not be considered a comprehensive source on hazard data. The function of the reported hazard data is to alert the user to possible hazards associated with the use of a

particular compound, but the absence of such data cannot be taken as an indication of safety in use, and the publishers cannot be held responsible for any inaccuracies in the reported information.

Many inorganic compounds have not been evaluated toxicologically but it is to be assumed that all compounds of certain elements such as As, Be, Hg and Tl are toxic, and that compounds containing certain groups such as perchlorate and azide are likely to be explosive.

The handling of many air-sensitive inorganic compounds is to be regarded as potentially hazardous because of the risk of fire or explosion in contact with air. Not every such compound has been specially marked as hazardous.

(*ii*) **Measures of toxicity.** Threshold limit values (TLV's) are a standard measure of the maximum permittable exposure without ill effects. They are issued annually by the American Conference of Governmental Industrial Hygienists (ACGIH), 6500 Glenway Avenue, Cincinnati, Ohio 45211, USA. Alternatively, Occupational Exposure Standards (OES's) for general reference to concentrations of toxic substances in air, and issued annually by the Health and Safety Executive, London, may be quoted, either in ppm (v/v) or mg m^{-3}.

(*iii*) **RTECS Accession Numbers.** Many entries contain one or more RTECS Accession Numbers. Possession of these numbers allows users to locate toxicity information on relevant substances from the NIOSH Registry of Toxic Effects of Chemical Substances.

The Registry is a compendium of toxicity data extracted from the scientific literature and each substance is identified by a unique nine-character alphanumeric RTECS Accession Number.

For each RTECS Accession Number the RTECS database provides the following data when available: substance name and synonyms; update date; CAS Registry Number; molecular weight and formula; reproductive, tumorigenic, and toxic dose data; and citations to aquatic toxicity ratings, IARC reviews, ACGIH Threshold Limit Values, toxicological reviews, existing Federal standards, the NIOSH criteria document program for recommended standards, the NIOSH current intelligence program, the NCI Carcinogenesis Testing Program, and the EPA Toxic Substances Control Act inventory.

RTECS is available in the following forms:

(*a*) Printed version (new edition annually) available from: Superintendent of Documents, U.S. Government Printing Office, Washington DC 20402.

(*b*) Microfiche edition (published quarterly), also available from U.S. Government Printing Office.

(*c*) RTECS on-line data base (updated quarterly), available from two sources: National Library of Medicine (NLM) Medical Literature Analysis and Retrieval System (MEDLARS), National Library of Medicine, 8600 Rockville Pike, Bethesda, Maryland 20209, and the National Institutes of Health/Environmental Protection Agency Chemical Information System (CIS), 2135 Wisconsin Avenue, NW, Washington, DC 20007.

(*d*) RTECS computer tape (produced annually), available from: National Technical Information Service (NTIS), Port Royal Road, Springfield, VA 22161.

5.11 *Bibliographic References*

The selection of references is made with the aim of facilitating entry into the literature for the user who wishes to locate more detailed information about a particular compound. Thus in general, recent references are preferred to older ones. The number of references quoted cannot be taken as an indication of the relative importance of a compound.

The contents of many references are indicated by means of abbreviated suffixes, of which the following are the most important:

(abs config)	absolute configuration
(anal)	analysis
(bibl)	bibliography
(biochem)	biochemistry
(biodistrbn)	biodistribution
(cd)	circular dichroism
(chromatog)	chromatography
(cmr)	carbon (^{13}C) nuclear magnetic resonance spectrum
(conformn)	conformation
(cryst struct)	x-ray crystal structure determination
(deriv)	reference referring to a derivative
(dsc)	differential scanning calorimetry
(ed)	electron diffraction
(electrochem)	electrochemistry
(em)	electron microscopy
(esr)	electron spin (paramagnetic) resonance spectrum
(formn)	formation
(glc)	gas–liquid chromatography
(haz)	hazard
(hplc)	high performance liquid chromatography

(ir)	infrared spectrum
(isom)	isomerism, isomerisation
(manuf)	manufacture
(mcd)	magnetic circular dichroism
(mineral)	mineralogy
(mord)	magnetic optical rotatory dispersion
(ms)	mass spectrum
(nd)	neutron diffraction
(nmr)	nuclear magnetic resonance spectrum
(nqr)	nuclear quadrupole resonance spectrum
(occur)	occurrence (minerals)
(ord)	optical rotary dispersion
(pe)	photoelectron spectrum (including x-ray photoelectron spectrum)
(pharmacol)	pharmacology
(photol)	photolysis
(pmr)	proton (^{1}H) nuclear magnetic resonance spectrum
(polarog)	polarography
(props)	properties (chemical or physical)
(purif)	purification
(rel compd(s))	related compounds
(resoln)	resolution
(rev)	review
(soly)	solubility
(struct)	structure
(synth)	synthesis
(tga)	thermogravimetric analysis
(thermol)	thermolysis
(thermodyn)	thermodynamic data
(tox)	toxicity
(trans)	transition(s)
(use(s))	use(s), application(s)
(uv-vis)	ultraviolet-visible spectrum

5.12 *Journal abbreviations*

In general these follow the practice of the *Chemical Abstracts Service Source Index* (CASSI) with one or two exceptions such as *Chemical Communications* published by the Royal Society of Chemistry. This changed its name from *Chem. Commun.* to *J. Chem. Soc. D* in 1970, then again to *J. Chem. Soc. Chem. Commun.* in 1972. For consistency the latter form has been used throughout.

In patent references, no distinction is made between patent applications and granted patents.

5.13 *Abbreviations*

[α]	specific rotation
abs. config.	absolute configuration
Ac	acetyl
acac	acetylacetonato
AcOH	acetic acid
alk.	alkaline
amorph.	amorphous
anal.	analytical applications, analysis or detection
anhyd.	anhydrous
approx.	approximately
aq.	aqueous
asym.	asymmetrical, unsymmetrical
B.	base
bibl.	bibliography
biosynth.	biosynthesis
bipy	2,2′-bipyridine
Bp	boiling point
c.	concentration
cmr	^{13}C nuclear magnetic resonance spectrum
ca.	(circa) about
c.d.	circular dichroism
chromatog.	chromatography
col.	colour, coloration
comly.	commercially
compd.	compound
conc.	concentrated, concentration
config.	configuration
constit.	constituent
coord.	coordination, coordinated
d.	density
dec.	decomposes, decomposition
deg.	degree
deriv(s).	derivative(s)
descr.	described
detn.	detection, determination
diars	diarsine (generalized ligand)
dil.	dilute, dilution
dimorph.	dimorphic
diphos	diphosphine (generalized ligand)
diss.	dissolves, dissolved
dist.	distil, distillation
DMA	dimethylacetamide
DMF	dimethylformamide
dmpe	1,2-bis(dimethylphosphino)ethane
dmpm	bis(dimethylphosphino)methane
dppe	1,2-bis(diphenylphosphino)ethane
dppm	bis(diphenylphosphino)methane
edta	ethylenediaminetetraacetato
E_g	band gap (electron volts)
en	ethylenediamine
equilib.	equilibrium
esp.	especially
esr	electron spin resonance spectrum
Et	ethyl
EtOAc	ethyl acetate
evapn.	evaporation

exp.	exposure, experimental
fl. p.	flash point
fluor.	fluoresces, fluorescence
formn.	formation
Fp	freezing point
ΔG_f°	standard free energy of formation
glc	gas liquid chromatography
haz.	hazard
ΔH_f°	standard enthalpy of formation
hplc	high performance liquid chromatography
hydrol.	hydrolyses, hydrolysed, hydrolysis
insol.	insoluble
ir.	infrared spectrum
isol.	isolated
J	Joules (energy)
K	Kelvin (temperature)
L	ligand
LD	lethal dose: LD50, a dose which is lethal to 50% of the animals tested
lit.	literature
M	metal
M	molar
manuf.	manufacture, manufactured
max.	maximum
Me	methyl
misc.	miscible
mixt.	mixture
mod.	moderately
mol.	mole(s)
Mp	melting point
ms	mass spectrum
n	index of refraction e.g. (n_D^{20} for 20° and sodium light)
nmr	nuclear magnetic resonance spectrum
nqr	nuclear quadrupole resonance spectrum
obt.	obtained
O_h	octahedral
oep	octaethylporphyrinato
OES	occupational exposure standard
ord.	optical rotatory dispersion
ox	oxalato
oxidn.	oxidation
pet. ether	petroleum ether (light petroleum)
Ph	phenyl (C_6H_5)
pharmacol.	pharmacology
phen	1,10-phenanthroline
pm	picometres (10^{-12} metre)
pmr	proton magnetic resonance spectrum
polarog.	polarography
porph	porphyrinato (generalized ligand)
pptd.	precipitated
prob.	probably
props.	properties
purifn.	purification
Py	pyridine
redn.	reduction
ref.	reference
resoln.	resolution
rev.	review
r.t.	room temperature
S°	standard entropy
sepn.	separation
sl.	slightly
sol.	soluble
soln.	solution
solv.	solvent
spar.	sparingly
struct.	structure
subl.	sublimation
synth.	synthesis
tautom.	tautomerism
THF	tetrahydrofuran
tbp	trigonal bipyramidal
T_d	tetrahedral
temp.	temperature
tlc	thin layer chromatography
tox.	toxicity
TLV	Threshold Limit Value
tpp	5,10,15,20-tetraphenylporphyrinato
μ_{eff}	effective magnetic moment (in Bohr magnetons μ_B)
unsatd.	unsaturated
uv	ultraviolet spectrum
v.	very
var.	variety
vis.	visible
vol.	volume
X	anion (usually halide)

6. Sources of further information

The following books and review series provide more information about various aspects of inorganic chemistry.

General

Gmelins Handbuch der Anorganischen Chemie, 8th Edn., Springer-Verlag, Berlin, 1922–

Mellor, J.W., *Comprehensive Treatise on Inorganic and Theoretical Chemistry*, Longman, London, 1922–

Advances in Inorganic Chemistry and Radiochemistry, Academic Press, N.Y., 1959–

Progress in Inorganic Chemistry, Interscience, 1959–

Progress in Solid State Chemistry, Pergamon, Oxford, 1964–

Transition Metal Chemistry, Marcel Dekker Inc., N.Y., 1965–

Coordination Chemistry Reviews, Elsevier, 1966–

Inorganic Reaction Mechanisms, Royal Society of Chemistry, London, 1971–

Inorganic Chemistry of the Transition Elements, Royal Society of Chemistry, London, 1972–

Comprehensive Inorganic Chemistry, Trotman-Dickinson, A.F. *et al*, Eds., Pergamon, Oxford, 1973.

Advances in Inorganic Biochemistry, Elsevier, 1977–

Kirk-Othmer Encyclopedia of Chemical Technology, 3rd Edn., Wiley, N.Y., 1978–1984.

Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1984.

The Chemistry of the Actinide Elements, 2nd Edn., Katz, J.J. *et al*, Eds., Chapman and Hall, 1986.

Comprehensive Coordination Chemistry, Wilkinson, G. *et al*, Eds., Pergamon, Oxford, 1987.

Cotton, F.A. *et al*, *Advanced Inorganic Chemistry*, 5th Edn., Wiley-Interscience, 1988.

Structures

Wyckoff, R.W.E., *Crystal Structures*, 2nd Edn., Wiley-Interscience, 1963–71.

Wells, A.F., *Structural Inorganic Chemistry*, 5th Edn., Oxford Science, 1984.

Smithells, C.J. *Metals Reference Book*, Plenum Press, N.Y., 1975.

Meyer, W.H., *et al*, *Atlas of Zeolite Structure Types*, 2nd Edn., Butterworths, London, 1987.

International Tables for X-Ray Crystallography, The International Union of Crystallography, London, 1952.

Minerals

Dana, J.D., *System of Mineralogy*, 7th Edn., Wiley, N.Y., 1944.

Encyclopedia of Minerals, 2nd Edn., Roberts, W.I., *et al* Eds., Van Nostrand Reinhold, N.Y., 1990.

Nomenclature

Nomenclature of Inorganic Chemistry, Leigh, G.J. *et al* Eds., IUPAC, Blackwell Scientific, Oxford, 1990.

Synthesis

Brauer, G., *Handbuch Präp. Anorganische Chemie*, 3rd Edn., Ferdinand Enke Verlag, 1975–81.

Inorganic Syntheses, Wiley-Interscience, 1939–

Toxicology

Doull, J. *et al*, *Toxicology*, 3rd Edn., Macmillan, N.Y., 1986.

Ac–C10

Ac IC-000001

Actinium

[7440-34-8]

Ac

M 227.0

Atomic No. 89. Ground state electron config. [Rn]$6d^17s^2$. 24 Isotopes reported: 2 occur naturally, of which ^{227}Ac is the most important ($t_{\frac{1}{2}}$ 21.8 years). Atomic radius 188 pm. Chemistry v. similar to that of La. Fcc struct. ^{227}Ac prepd. by neutron bombardment of ^{226}Ra. Metal obt. from AcF_3 or Ac_2O_3 + Li in Mo crucible at 1100-1300°, or from $AcCl_3$ + K. ^{227}Ac considered as a heat source in thermoelectric generators (for interplanetary flight). Soft silvery white metal, sometimes with golden caste, which glows in the dark. Oxidised rapidly (→ Ac_2O_3) in moist air. Reacts with H_2O (→ H_2). Mp *ca.* 1050° (1430°). Bp *ca.* 3200° (est.). ^{227}Ac is a member of the ^{235}U (AcU) decay series.

▷ ^{225}Ac is an α-emitter. ^{227}Ac is a weak β-emitter.

[14265-85-1, 14331-83-0, 14952-40-0]

Gmelin Handbook Inorg. Chem., Syst. No. 40, 1942; *Suppl. Vol.* 1, 1981 (*rev, bibl*)
Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 803 (*history*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **5**, 5 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1117.
Keller, C., *Chem.-Ztg.*, 1977, **101**, 500 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **19**, 639, 682 (*rev, bibl*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 1450 (*rev*)
Kirby, H.W., *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, **1**, 14 (*rev, bibl*)
Stirlet, J.C. *et al*, *Adv. Inorg. Chem.*, 1987, **31**, 1 (*rev, bibl*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 12 (*data*)

AcBrO IC-000002

Actinium(*III*) bromide oxide (AcBrO)

Actinium(III) *oxybromide*

[49848-33-1]

AcOBr

M 322.9

Possesses the PbClF or BiOCl struct. with 8-coord. Ac. White solid.

Zachariasen, W.H., *Acta Crystallogr.*, 1949, **2**, 388 (*struct*)
Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)
Moskvin, A.I., *Radiokhimiya*, 1973, **15**, 353, 362; *CA*, **79**, 97595, 97596.

$AcBr_3$ IC-000003

Actinium(*III*) bromide ($AcBr_3$)

Actinium tribromide

[33689-81-5]

$AcBr_3$

M 466.7

Possesses the UCl_3 struct. Synth. from Ac_2O_3 + $AlBr_3$ (750°). White solid. Sol. H_2O. Subl. 800°. ΔH_f° −843 kJ mol^{-1}.

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*cryst struct*)
Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)
Finogenov, A.D., *Zh. Fiz. Khim.*, 1971, **45**, 1586; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1971, **45**, 900.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1126 (*synth*)
Bratsch, S.G. *et al*, *J. Phys. Chem.*, 1986, **90**, 207.

AcClO IC-000004

Actinium(*III*) chloride oxide (AcClO)

Actinium(III) *oxychloride*

[49848-29-5]

AcOCl

M 278.4

Possesses the PClF or BiOCl struct. with 8-coord. Ac. White solid.

Zachariasen, W.H., *Acta Crystallogr.*, 1949, **2**, 288 (*struct*)
Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)

$AcCl_3$ IC-000005

Actinium(*III*) chloride ($AcCl_3$)

Actinium trichloride

[22986-54-5]

$AcCl_3$

M 333.3

Possesses the UCl_3 struct. Synth. from $Ac(OH)_3$ + CCl_4 (500°). White solid. Sol. H_2O. Subl. 960°. ΔH_f° −1011 kJ mol^{-1}.

[27388-90-5]

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*cryst struct*)
Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)
Merinis, J. *et al*, *Radiochem. Radioanal. Lett.*, 1970, **3**, 255.
Finogenov, A.D., *Zh. Fiz. Khim.*, 1971, **45**, 1586; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1971, **45**, 900.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1125 (*synth*)
Bratsch, S.G. *et al*, *J. Phys. Chem.*, 1986, **90**, 307.

AcFO IC-000006

Actinium(*III*) fluoride oxide (AcFO)

Actinium(III) *oxyfluoride*

[49848-24-0]

AcOF

M 262.0

Possesses the fluorite struct. White solid.

Zachariasen, W.H., *Acta Crystallogr.*, 1949, **2**, 388 (*struct*)
Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)

AcF_3 IC-000007

Actinium(*III*) fluoride (AcF_3)

Actinium trifluoride

[33689-80-4]

AcF_3

M 284.0

Possesses the LaF_3 struct. Synth. from $Ac(OH)_3$ + HF. White solid. Insol. H_2O. ΔH_f° −1624 kJ mol^{-1}.

Zachariasen, W.H., *Acta Crystallogr.*, 1949, **2**, 388 (*cryst struct*)
Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)
Finogenov, A.D., *Zh. Fiz. Khim.*, 1971, **45**, 1586; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1971, **45**, 900.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1124 (*synth*)
Bratsch, S.G. *et al*, *J. Phys. Chem.*, 1986, **90**, 307.

AcH_3O_3 IC-000008

Actinium(*III*) hydroxide ($Ac(OH)_3$)

Actinium trihydroxide

$Ac(OH)_3$

M 278.0

White solid. Insol. H_2O (3.6×10^{-6} g 100 cm^{-3}). Soly. altered on ageing.

Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)
Zin, D.M. *et al*, *Soc. Radiochem. (Engl. Transl.)*, 1965, **7**, 176 (*synth*)

AcI_3 IC-000009

Actinium(*III*) iodide (AcI_3)

Actinium triiodide

[35089-82-6]

AcI_3

M 607.7

White solid. Sol. H_2O. Subl. 700-800°. ΔH_f° −2533 kJ mol^{-1}.

Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth*)
Finegenov, A.D. *et al*, *Zh. Fiz. Khim.*, 1971, **45**, 1586; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1971, **45**, 900.
Bratsch, S.G. *et al*, *J. Phys. Chem.*, 1986, **90**, 207.

Ac_2O_3 IC-000010

Actinium(*III*) oxide (Ac_2O_3)

Diactinium trioxide. Actinium sesquioxide

[12002-61-8]

Ac_2O_3

M 502.0

Has rare-earth sesquioxide A-struct. Formed when metal oxidised and when the oxalate is heated. White solid. Insol. H_2O. Can be reduced to Ac.

[74238-81-6]

Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth, struct*)

Ac_2S_3 IC-000011

Actinium(*III*) sulfide (Ac_2S_3)

[50647-18-2]

Ac_2S_3

M 550.2

Isostructural with Ce_2S_3. Synth. from Ac_2O_3 + H_2S. Dark cubic cryst.

Fried, S. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 771 (*synth, struct*)

Ag IC-000012

Silver

Argentum (L.)

[7440-22-4]

Ag

M 107.8

Atomic No. 47. Ground state electron config. $[Kr]4d^{10}5s^1$. 27 Isotopes are known of which ^{107}Ag and ^{109}Ag are natural. Abundance: 0.08 ppm (earth's crust), 3×10^{-4} ppm (sea water). No biological role. Fcc struct. (Al type). Known to ancient civilizations. Occurs as natural metal, and as argentite (Ag_2S). Prod. as by-product from manuf. of non-ferrous metals, e.g. Cu, Pb, Zn. Excellent electrical and thermal conductor. Important compds. used in photography; used also in jewellery, electrical cells. Industrial catalyst. Soft malleable, ductile metal with silver sheen. Tarnishes in air with formation of black sulfide. Phys. props. dependent on mechanical treatment. Attacked by Cl_2, S, H_2S, metal cyanides (in air), chromic, nitric and sulfuric acids. Mp 961°. Bp 2163° (2155°). d^{25} 10.50 g cm^{-3}. Stable to O_2, and to H_2O, but attacked by S and its compds. and by $Cl^\ominus$. Sol. H_2SO_4, (hot, conc.) and HNO_3 (dil.). Sol. aq. $CN^\ominus$ solns. (+ H_2O_2).

▷ Toxic to lower organisms, but not mammals. Dust may be pyrophoric. VW3500000.

[14378-37-1, 14378-38-2]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1923, **3**, 295 (*res, bibl*)
Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 3 (*history*)
Gmelin Handbook Inorg. Chem., Syst. No. 61, 1970, **A1, A2**; 1971, **A3**; 1973, **A4** (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **3**, 79 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 993 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **21**, 1 (*res, bibl*)
Henrichs, P.M., *NMR Newly Accessible Nuclei*, (Ed. Laszlo, P.), Academic Press, N.Y., 1983, **2**, 319 (*Ag-109 nmr*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 1364 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 176.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 2 (*haz*)

[AgAl] IC-000013

Silver-aluminium system

Aluminium-silver system

Several alloys known.

***Silver aluminium* (*3:1*)** [11089-73-9]

Ag_3Al M 350.5

β'-form (sometimes designated μ) has the β-Mn type struct.; the β-form has a ccp disordered struct.

***Silver aluminium* (*2:1*)** [12249-71-7]

γ-Silver-aluminium

Ag_2Al M 242.7

hcp struct.

Westgren, A. *et al*, *Philos. Mag.*, 1928, **6**, 280 (Ag_3Al, *struct*)
Hofmann, W. *et al*, *Metallwiss., Metalltech.*, 1936, **15**, 699 (Ag_3Al, *struct*)
Morris, D.P. *et al*, *Acta Crystallogr.*, 1961, **14**, 74 (Ag_3Al, *struct*)
Neumann, J.P. *et al*, *Trans. Metall. Soc. AIME*, 1968, **242**, 700 (Ag_2Al, *struct*)
Nemnonov, S.A. *et al*, *J. Phys. Colloq.*, 1971, 307 (Ag_2Al, *x-ray spec*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)
Karlsson, U.O. *et al*, *Surf. Sci.*, 1983, **126**, 58 (Ag_2Al, *pe*)

$AgAsF_6$ IC-000014

Silver(1+) hexafluoroarsenate, 9CI

[12005-82-2]

$Ag[AsF_6]$

M 296.7

Prepd. from Ag + AsF_5 in liq. SO_2 or from Ag + As_2O_3 + BrF_3. Commercially available. White cryst., sensitive to moisture and light. V. sol. SO_2; insol. nonpolar solvs.

Woolf, A.A. *et al*, *J. Chem. Soc.*, 1950, 1050 (*synth*)
Cox, B. *et al*, *J. Chem. Soc.*, 1956, 876 (*cryst struct*)

Pitts, J.J. *et al*, *Inorg. Chem.*, 1965, **4**, 257 (*ir*)
Guo, Q.Z. *et al*, *J. Magn. Reson.*, 1984, **57**, 143 (*F-19 nmr*)
Inorg. Synth., 1986, **24**, 72 (*synth*)

$AgAsPbS_3$ IC-000015

Marrite

Lead silver arsenide sulfide ($PbAgAsS_3$)

[12211-36-8]

$AgPbAsS_3$

M 486.1

Arsenic is coord. by 3 nearest S neighbours to give trigonal pyramid. Ag coord. by 3 nearest S neighbours to give near planar arrangement. Pb coord. by 6 nearest S neighbours to give an irregular octahedron. Lead grey to steel grey metallic cryst.

Wuensch, B.J. *et al*, *Z. Kristallogr.*, 1967, **125**, 459 (*cryst struct*)
Maijs, L., *Latv. PSR Zinat. Akad. Vestis, Khim. Ser.*, 1979, 11.
Nakai, I. *et al*, *Proc. Int. Symp. Hydrotherm. React. (1st, 1982)*, 1982, 772 (*synth*)

$AgAuTe_4$ IC-000016

Gold silver telluride ($AuAgTe_4$)

[102430-10-4]

$AuAgTe_4$

M 815.2

Cryst. with metallic lustre, electrically conducting. Brittle.

Mineral-form

Sylvanite

Widespread occurrence in low to high temp. vein deposits commonly associated with other minerals. Silver-white monoclinic cryst. sometimes with yellowish tint. Very similar structurally to $(Au,Ag)Te_2$ calavarite and krennerite.

Tunnell, G. *et al*, *Acta Crystallogr.*, 1952, **5**, 375 (*cryst struct*)
Langouche, G. *et al*, *Hyperfine Interact.*, 1986, **28**, 849 (*mössbauer*)

$AgBF_4$ IC-000017

Silver(1+) tetrafluoroborate

Silver fluoboride

[14104-20-2]

$Ag[BF_4]$

M 194.6

Prepd. by reaction of BF_3 with AgF in $MeNO_2$ or C_6H_6. Catalyst in org. synthesis. Commercially available. White cryst. Deliquescent. V. sol. H_2O, Et_2O, toluene, $MeNO_2$; mod. sol. C_6H_6, cyclohexene; insol. cyclohexane.

▷ Poisonous. ED2875000.

Sharpe, A.G., *J. Chem. Soc.*, 1952, 4538 (*synth*)
Olah, G.A. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **14**, 295 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1015 (*synth, use*)
Clark, J.B. *et al*, *Z. Phys. Chem. (Frankfurt am Main)*, 1974, **88**, 242 (*cryst struct, polymorphism*)
Sears, R.E.J., *J. Chem. Phys.*, 1980, **72**, 2888 (*F-19 nmr*)
Padma, D.K., *Synth. React. Inorg. Metal-Org. Chem.*, 1988, **18**, 401 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3028.

[AgBe] IC-000018

Silver-beryllium system

Beryllium silver

Alloy.

***Silver beryllium* (*1:2*)**

$AgBe_2$ M 125.8

$MgCu_2$-type struct. Metallic.

Misch, L., *Metallwiss., Metalltech.*, 1936, **15**, 163 (*struct*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

AgBr IC-000019

Silver(*I*) bromide (AgBr)

[7785-23-1]

AgBr

M 187.7

NaCl struct. Used in photography. Commercially available. Yellowish, odourless powder. Darkens on exp. to light. Insol. alcohols, most acids; mod. sol. conc. aq. ammonia; sol. solns. of alkali cyanides. Mp 430°. Bp 1533°. ΔH_f° −99.5 kJ mol^{-1}, ΔG_f° −96.3 kJ mol^{-1}.

Jost, W. *et al*, *Z. Phys. A:*, 1936, **B34**, 348 (*conductivity*)
Gurney, R.W. *et al*, *Proc. R. Soc. London, A*, 1938, **164**, 151 (*use*)
Martin, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1945, **220**, 659 (*anal*)
Sathe, N.V. *et al*, *J. Indian Chem. Soc.*, 1945, **22**, 29 (*props*)
Takahashi, H. *et al*, *J. Phys. Soc. Jpn.*, 1987, **56**, 3593 (*cryst struct, synth*)
Merck Index, 11th Ed., 1989, No. 8452.

[AgCa] IC-000020

Calcium-silver system

Silver-calcium system

Alloy; two phases descr. here.

***Calcium silver* (*1:2*)** [12399-39-2]

Ag_2Ca M 255.8

Has $MgZn_2$-type struct. Metallic.

***Calcium silver* (*5:3*)** [12399-40-5]

Ag_3Ca_5 M 523.9

Metallic.

Rand, R.P. *et al*, *Can. J. Chem.*, 1962, **40**, 705 (Ag_3Ca_5, *struct*)
Alexander, W.A. *et al*, *Can. J. Chem.*, 1969, **47**, 611 (*phase diagram*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

[AgCd] IC-000021

Silver-cadmium system

Cadmium-silver system

***Silver cadmium* (*1:1*)** [12002-62-9]

AgCd M 220.2

β-form: Stable above 443°. A2 (W-type) struct.-ccp.

β_1-form: ζ-AgCd

Stable between 186 and 475°. A3 (Mg-type) struct.-hcp.

β'-form: Stable below 210°. B2 (CsCl-type) struct.

***Silver cadmium* (*5:8*)** [61104-55-0]

γ-Silver-cadmium

Ag_5Cd_8 M 1438.6

Struct. similar to γ-brass.

***Silver cadmium* (*1:3*)** [39399-53-6]

ε-Silver-cadmium

$AgCd_3$ M 445.1

Hcp struct.

Wollen, E.O., *Phys. Rev.*, 1934, **53**, 203 ($AgCd_3$, *struct*)
Owens, E.A. *et al*, *J. Inst. Met.*, 1939, **65**, 457 (Ag_5Cd_8, *struct*)

Muldawer, L. *et al*, *Trans. Am. Inst. Min., Metall. Pet. Eng.*, 1953, **197**, 1458 (*AgCd, struct*)
Mansfield, T.B., *J. Inst. Met.*, 1959, **88**, 232 (*AgCd, struct*)
Quader, A., *Indian J. Phys.*, 1960, **34**, 506 (*AgCd, struct*)
Ahrista, J.P. *et al*, *Sov. Metall.*, 1968, **2**, 41 (*AgCd, struct*)
Haas, H. *et al*, *J. Chem. Phys.*, 1973, **58**, 3339 (*AgCd$_n$, mgr*)
Kaul, P.H. *et al*, *J. Phys. Chem.*, 1978, **82**, 1554 (*AgCd, esr*)
Wertheim, G.K. *et al*, *Phys. Rev. B: Condens. Matter*, 1979, **20**, 860 (*AgCd, pe*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

AgCe — IC-000022

Cerium silver (1:1)
Silver cerium (AgCe)
[12040-88-9]

AgCe

M 247.9
Alloy with CsCl-type struct. above 16K and tetragonal struct. below 16K. Only ferromagnetic compd. among the rare earth-silver compds.: T_c 5.5K. Metallic.

Dwight, A.E., *U.S. At. Energy Comm.*, ANL-6099, 1959, 94 (*struct*)
Wallace, R.E. *et al*, *J. Chem. Phys.*, 1964, **41**, 3285 (*magnetism*)
Kadomatsu, H. *et al*, *Phys. Lett. A*, 1979, **70**, 472 (*magnetism*)
Takle, R. *et al*, *J. Magn. Magn. Mater.*, 1981, **23**, 247 (*magnetism*)
Fujiwara, H., *Physica B+C (Amsterdam)*, 1983, **119**, 142 (*magnetism, rev*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

AgCl — IC-000023

Silver(*I*) chloride (AgCl)
Argentous chloride
[7783-90-6]

AgCl

M 143.3
NaCl struct. Used in silver plating and in making antiseptic silver preparations. Commercially available. White powder. Darkens on exp. to light. Spar. sol. H_2O; sol. conc. NH_3, alkali cyanides; insol. dil. acids, EtOH. Mp 455°. Bp 1550°. ΔH_f° −127.3 kJ mol^{-1}.

Tubandt, C. *et al*, *Z. Phys. A.*, 1922, **100**, 489 (*conductivity*)
Barth, T. *et al*, *Z. Phys. A.*, 1926, **122**, 293 (*cryst struct*)
Pauling, L., *Phys. Rev.*, 1929, **34**, 959 (*magnetism*)
Derr, P.F. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 2670 (*synth*)
Chaléroux, C., *Ann. Chim.*, 1960, **5**, 1069 (*synth*)
Alexander, R. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 3703 (*soly*)
Schock, R.N. *et al*, *J. Phys. Chem. Solids*, 1969, **30**, 1527 (*high pressure structs*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 995.
Inorg. Synth., 1980, **20**, 18 (*synth*)
Merck Index, 11th Ed., 1989, No. 8455.

$AgClO_3$ — IC-000024

Silver(*I*) chlorate(*V*) ($AgClO_3$)
Argentous chlorate
[7783-92-8]

$AgClO_3$

M 191.3
Oxidising agent for some organic syntheses. White, tetragonal cryst. Darkens upon exp. to light due to slow dec. Spar. sol. H_2O; sl. sol. alcohols. Mp 230°. Dec. at 270° forming silver chloride and oxygen.

Hendrixson, W.S., *J. Am. Chem. Soc.*, 1903, **25**, 637 (*synth*)
Braun, G., *J. Am. Chem. Soc.*, 1929, **51**, 228 (*use*)
Natay-Szabo, S. *et al*, *Z. Kristallogr.*, 1942, **104**, 28 (*cryst struct, synth*)
Inorg. Synth., 1946, **2**, 4 (*synth, props*)
Merck Index, 11th Ed., 1989, No. 8454.

$AgClO_4$ — IC-000025

Silver(*I*) perchlorate ($AgClO_4$)
[7783-93-9]

$AgClO_4$

M 207.3
Struct. unique for perchlorates of monovalent cations: tetragonal with 4+4 coordination at silver. Ag—O 250.4, 277.9 pm. Used in the explosives industry. Commercially available. Deliquescent cryst. Freely sol. H_2O; sol. C_6H_6, Py, toluene. Dec. at 486°.

▷ Irritating to skin, mucous membranes. Forms many explosive solvates.

Smith, G.F. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 1889 (*synth, props*)
Brinkley, S.R., *J. Am. Chem. Soc.*, 1940, **62**, 3524 (*synth, solvates, haz*)
Markowitz, M.M. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **16**, 159 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 997 (*synth*)
Berthold, H.J., *Z. Kristallogr.*, 1979, **149**, 327 (*cryst struct*)
Merck Index, 11th Ed., 1989, No. 8470.

$AgCrS_2$ — IC-000026

Chromium silver sulfide ($CrAgS_2$)
Silver chromium sulfide ($AgCrS_2$). Silver thiochromite
[12249-43-3]

$AgCrS_2$

M 223.9
Prepd. by heating Ag_2S + Cr_2S_3. Commercially available. Soft, dark powder.

Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1957, **290**, 68 (*synth*)
Vallet, E. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **264**, 772 (*synth*)
Engelsman, F. *et al*, *J. Solid State Chem.*, 1973, **6**, 574 (*cryst struct*)

[AgCu] — IC-000027

Copper-gold system
Gold copper

Copper gold (1:1) [12006-51-8]
AuCu M 260.5
Has fcc superstruct. of the Cu type below 380° with layers of Cu and Au. Disordered above 420°.

Copper gold (3:1) [12006-52-9]
Au_3Cu M 654.4
High temp. struct. is fcc with disorder between Cu and Au. Low temp. struct. is similar but with ordered Au and Cu.

Hansson, B. *et al*, *Acta Metall.*, 1964, **12**, 315 (*struct, CuAu*)
Schubert, K., *Metall (Berlin)*, 1966, **20**, 424 (*rev*)
Bjerkelund, E. *et al*, *Acta Chem. Scand.*, 1967, **21**, 2900 (*cryst struct, CuAu*)
Gavert, R.D. *et al*, *Trans. Metall. Soc. AIME*, 1967, **239**, 130 (*phys prop, CuAu*)
Dirand, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **280**, 559 (*struct, CuAu*)
Lander, G.H. *et al*, *J. Phys. C*, 1982, **15**, 6699 (*nd*)
Bogdanov, V.I. *et al*, *Phys. Status Solidi B*, 1982, **110**, 431 (*theory*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

Jordan, R.G., *High Temp. Alloys: Theory Des. (Proc. Conf.)*, 1984, 39 (*pe, rev*)
Fox, A.G., *Philos. Mag., Part B*, 1984, **50**, 477 (*struct, Cu_3Au*)
Jordan, R.G. *et al*, *J. Phys., (France)*, 1985, **15**, L135 (*photoemission*)
Eberhardt, W. *et al*, *Phys. Rev. B: Condens. Matter*, 1985, **31**, 8285 (*electronic struct, Cu_3Au*)

AgF — IC-000028

Silver(*I*) fluoride (AgF)
Argentous fluoride. Silver monofluoride
[7775-41-9]

AgF

M 126.8
NaCl struct. Converts organic Br and Cl compds. into their F analogues; antiseptic. Commercially available. V. hygroscopic leaflets. Darkens on exp. to light. Sol. H_2O, HF, NH_3, MeCN. Mp 435°. Bp 1150°. In moist air becomes insol. in H_2O due to the formation of the basic fluoride. Reduced to the subfluoride by uv light. ΔH_f° −203.7 kJ mol^{-1}.

Dihydrate: Stable to 39.5°.
Tetrahydrate: Stable from −14° to +18.7°.

Ott, H., *Z. Kristallogr.*, 1926, **63**, 222 (*cryst struct*)
Jahn-Held, W. *et al*, *Z. Elektrochem.*, 1936, **42**, 608 (*hydrate*)
Freed, S. *et al*, *J. Chem. Phys.*, 1940, **8**, 225 (*magnetism*)
McCaulay, D.A. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 2495 (*use*)
Abragam, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **249**, 1633 (*Ag-109 nmr*)
Ladd, M.F. *et al*, *J. Inorg. Nucl. Chem.*, 1959, **11**, 264 (*theory*)
Won Choi, Q., *J. Am. Chem. Soc.*, 1960, **82**, 2686 (*F-19 nmr*)
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, 240 (*synth*)
Merck Index, 11th Ed., 1989, No. 8460.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3030.

AgF_2 — IC-000029

Silver(*II*) fluoride (AgF_2)
Argentic fluoride. Silver difluoride
[7783-95-1]

AgF_2

M 145.8
The only known binary Ag(*II*) compd. Struct. comprises distorted hcp fluoride with Ag(*II*) arranged on fcc sites. Commercially available. V. hygroscopic; white when pure. Usually obt. as a grey-black or brownish amorphous solid. Light sensitive.

▷ Highly toxic. Violent reaction with water. Powerful oxidising agent. VW4200000.

Ebert, M.S. *et al*, *J. Am. Chem. Soc.*, 1933, **55**, 3056 (*synth*)
Ruff, O. *et al*, *Z. Anorg. Allg. Chem.*, 1934, **219**, 143 (*synth, cryst struct*)
Inorg. Synth., 1950, **3**, 176 (*synth*)
Rochow, E.G. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 1615 (*synth*)
Fischer, P. *et al*, *J. Phys. Chem. Solids*, 1971, **32**, 543 (*nd*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 248 (*synth*)
Merck Index, 11th Ed., 1989, No. 8459.

AgF_3Zn — IC-000030

Silver zinc fluoride ($AgZnF_3$)
Silver trifluorozincate
[28667-89-2]

$AgZnF_3$

M 230.2
Perovskite struct. Cryst.

Porties, J. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **270**, 216 (*synth, struct*)
Beznosikov, B.V., *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1978, **23**, 51 (*cryst struct*)

$AgF_4^{\ominus}$ — IC-000031

Tetrafluoroargentate(*III*)(1−)
[91899-67-1]

$[AgF_4]^{\ominus}$

M 183.8 (ion)
Square planar at Ag. Fluorinating agent.

Na salt: [31096-68-1].
AgF_4Na M 206.8
Yellow cryst.

K salt: [23739-18-6]. *Potassium tetrafluoroargentate ($KAgF_4$)*
AgF_4K M 222.9
Yellow cryst.

Hoppe, R., *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1956, **75**, 569 (*synth, anal, magnetism*)
Hoppe, R. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **379**, 193 (*cryst struct*)
Edwards, A.J. *et al*, *J. Fluorine Chem.*, 1971, **1**, 246 (*cryst struct*)

AgF_5OTe — IC-000032

|Pentafluorohydroxytellurato(1−)|silver
Silver teflate. Silver pentafluoroorthotellurate. Silver(1+) pentafluorooxotellurate, 9CI
[50700-88-4]

$AgOTeF_5$

M 346.4
The various solvates with aromatics and halocarbons contain coordinated solv. molecules and offer an entry into reactive solvated metal ion chemistry. Synth. from AgF + TeF_5OH in presence of required solv. Grey powder. Extremely sol. CH_2Cl_2, 1,2-dichloroethane (> 2.5*M*).

CH_2Cl_2 complex: [116909-86-5].
White powder; dec. slowly in light at r.t. Sol. CH_2Cl_2.

1,2-Dichloroethane complex: see *Bis(1,2-dichloroethane-Cl,Cl')bis[μ-[pentafluorohydroxytellurato(1−)-O:O]] disilver(I), IC-004049*

Bis-MeCN complex: [98330-70-2]. *Tetrakis(acetonitrile-N) bis[μ-[pentafluorohydroxytellurato(1−)-O:O]]disilver, 9CI*
Sticky white solid. Dimeric.

Bis-toluene complex: [98330-69-9].
White cryst. stable indefinitely in dark at −15°. Dimeric.

Mayer, E. *et al*, *Inorg. Chem.*, 1975, **14**, 589 (*synth, MeCN complex*)
Strauss, S.H. *et al*, *Inorg. Chem.*, 1985, **24**, 4307 (*complexes, synth, F-19 nmr, cryst struct*)
Colsman, M.R. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6886 (*synth, CH_2Cl_2 complex*)

$AgF_6^{3\ominus}$ — IC-000033

Hexafluoroargentate(*III*)(3−)

$[AgF_6]^{3\ominus}$

M 221.8 (ion)
The first known Ag^{III} salt with 6-coordination.

K alt-(C) salt [74480-87-0]
AgO_2F_4K M 326.7
Obt. by direct fluorination of a 2:1 mixt. of CsCl, KCl, $AgNO_3$ at 300°. Unstable purple-red cryst. Struct. resembles K_2NaOrF_6, cubic.
Bojan, B. et al, Magnetochemistry, 1986, 83, 501 (comb. anal., magnetism, cryst. struct.)
Allen, G.C. et al, Inorg. Chem., 1988, 8, 1895 (ir-vis)

IC-000034

AgF_4^{-}
Hexafluoroargentate(III,IV)(2−)
$[AgF_4]^{\ominus}$ $[AgF_4]^{\ominus}$
M 227.8 (ion)
Mixed valence state Ag^{II}/Ag^{III} compd. with D_4 Ag.
Di-Cs salt: [82388-00-5]
$AgCs_2F_8$ M 487.6
Obt. by heating a 2:1 mixt. of CsF and AgF_2. Bright orange cryst. Dec. in air/water; loses fluorine at r.t. in vacuo. Made up of equal amts. of Ag^{III} and Ag^{I} in the cryst. lattice.
Serbe, P. et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C, 1977, 284, 231 (synth, cryst struct, magnetism)
Serbe, P. et al, J. Fluorine Chem., 1978, 11, 243 (synth, cryst struct, magnetism)

IC-000035

AgF_6P
Silver(1+) hexafluorophosphate
[26042-63-7]
$Ag[PF_6]$
M 252.8
Prepd. from AgF + PF_5 in liq. SO_2. Commercially available. Yellow-brown solid. Sol. H_2O.
Woolf, A.A. et al, J. Chem. Soc., 1950, 1050 (synth)
Russell, D.R. et al, J. Chem. Soc., 1961, 4689 (synth)
Emeléus, R.D.W. et al, J. Chem. Soc., 1963, 4408 (cryst struct)

IC-000036

$AgFe_2S_3$
Iron silver sulfide (Fe_2AgS_3)
Argentopyrite
[12417-96-8]
$AgFe_2S_3$
M 315.7
Mineral. Grey to white with metallic lustre. Dimorphous with Sternbergite.
Murdoch, J. et al, Am. Mineral., 1954, 39, 475 (struct)
Sventsitskaya, O.L. et al, Nov. Dannye Miner., 1982, 30, 135; CA, 1983, 99, 41172s (struct, reflectance)

IC-000037

[AgGa]
Silver-gallium system
Gallium silver system
Alloy; main phase is Ag_3Ga.
Silver gallium (3:1) [57673-43-7]
Ag_3Ga M 393.3
Exists in γ-phase below 440° and β-phase above this temp. The β-phase has a disordered Mg-like struct. (hcp) and is sometimes designated ζ or γ, ξ'. Metallic.
Hume-Rothery, W. et al, J. Inst. Met., 1942, 68, 133 (struct)
Hellner, E., Fortschr. Mineral., 1950, 29-30, 58 (struct)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (struct, props)

IC-000038

$AgH_4O_4^{\ominus}$
Argentate ($Ag(OH)_4^{\ominus}$)
Tetrahydroxoargentate(1−). Silver(III) tetrahydroxide(1−)
[25172-26-1]
$[Ag(OH)_4]^{\ominus}$
M 175.8 (ion)
Square planar Ag^{III} complex. Highly oxidising, metastable in aq. soln.
Cohen, G.L. et al, J. Electrochem. Soc., 1968, 115, 1236 (synth, electrochem)
Kirschenbaum, L.J. et al, Inorg. Chem., 1973, 12, 12 (synth, electrochem, uv, kinetics)
Kirschenbaum, L.J., J. Am. Chem. Soc., 1984, 106, 1003 (reactions)
Kirschenbaum, L.J. et al, Polyhedron, 1985, 4, 1573 (reactions)

IC-000039

$AgH_6N_2^{\oplus}$
Diamminesilver(1+), 11Cl, 10Cl, 9Cl, 8Cl
[16972-61-5]
$[H_3N{-}Ag{-}NH_3]^{\oplus}$
M 141.9 (ion)
Linear cation. Stain for DNA to detect aldehyde groups in deoxyribose function. Basis of Tollen's reagent used to test for the presence of aldehydes.
Perchlorate: [103809-62-7]. *Silver(I) perchlorate diammoniate*
White cryst.
▷ Potentially explosive.
Nitrate: [23606-32-8]. *Silver(I) nitrate diammoniate*
White cryst. Dec. in air with loss of NH_3 within a few hrs.
▷ VW3515000.
Miles, M.G. et al, Inorg. Chem., 1968, 7, 1721 (synth, raman, ir)
Geddes, A.L. et al, Inorg. Chem., 1969, 8, 802 (ir)
Maurer, H.M. et al, Z. Kristallogr., 1977, 146, 227 (cryst struct)
Maurer, H.M. et al, J. Chem. Phys., 1978, 69, 4046 (pmr)
Yamagachi, T. et al, Acta Chem. Scand., Ser. A, 1983, 37, 685 (cryst struct)
Nakatsuji, H. et al, J. Am. Chem. Soc., 1984, 106, 4653 (nmr)
Endo, K. et al, J. Magn. Reson., 1985, 65, 268 (Ag-109 nmr, uv)

IC-000040

[AgHg]
Mercury-silver system
Silver-mercury system. Silver amalgam
Silver mercury (3:4) [12250-07-6]
γ-Silver-mercury
Ag_3Hg_4 M 1125.9
Struct. similar to γ-brass.
Silver mercury (11:9)
ε-Silver-mercury
$Ag_{11}Hg_9$ M 2991.8
hcp struct.
Preston, G.D., J. Inst. Met., 1931, 46, 522 ($Ag_{11}Hg_9$, struct)
Westgren, A., J. Inst. Met., 1931, 46, 533 (Ag_3Hg_4, struct)
Ryge, G. et al, J. Dent. Res., 1953, 32, 152 (Ag_3Hg_4, struct)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (struct, props)

IC-000041

AgI
Silver(I) iodide (AgI)
[7783-96-2]
AgI
M 234.7

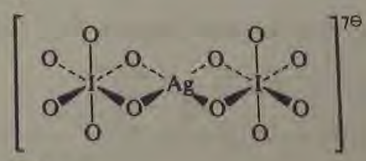
Possesses wurtzite struct. at r.t. which transforms to the fast silver ion conducting form at 147° which has bcc iodide. Another low temp. form has the sphalerite struct. NaCl struct. available only at elevated pressure. Used in cloud precipitation and as a local anti-infective. Commercially available. Light yellow odourless powder. Slowly darkens in light. Cryst. are hexagonal or cubic. Insol. H_2O, acids, ammonium carbonate; sol. aq. alkali cyanides and iodides. Mp 558°. Bp 1504°.
Cochrane, G., *Brit. J. Appl. Phys.*, 1967, **18**, 687 (*synth, single cryst*)
Takahashi, T., *J. Appl. Electrochem.*, 1973, **3**, 79 (*conductivity*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 995 (*synth*)
Wright, A.F. *et al*, *J. Phys. C*, 1977, **10**, 2271 (*cryst struct*)
Boyle, J.B. *et al*, *Phys. Rev. Lett.*, 1977, **38**, 1362 (*exafs*)
Cava, R.J. *et al*, *Solid State Commun.*, 1977, **24**, 411 (*nd*)
Wells, A.F., *Structural Inorg. Chem.*, 5th Ed. O.U.P., 1984, 410 (*struct*)
Merck Index, 11th Ed., 1989, No. 8462.

IC-000042

$AgIO_3$
Silver(*I*) iodate ($AgIO_3$)
Argentous iodate
[7783-97-3]
$AgIO_3$
M 282.7
IO_3 groups and AgO_6 octahedra form a compact 2-D framework. Isomorphous with $AgNO_3$ and $(NH_4)IO_3$. Reagent for determining small quantities of chloride. Commercially available. Light-sensitive white cryst. powder. Spar. sol. H_2O, HNO_3; mod. sol. 10% NH_3. ΔH_f° −95.8 kJ mol^{-1}. Dec. between 410-470°.
Hendrixson, W.S., *J. Am. Chem. Soc.*, 1903, **25**, 637 (*synth*)
Sendrog, J., *J. Biol. Chem.*, 1937, **120**, 335 (*synth*)
Dasent, W.E. *et al*, *J. Chem. Soc.*, 1960, 2429 (*ir*)
Pitts, J.J. *et al*, *Inorg. Chem.*, 1965, **4**, 257 (*ir*)
Pacesova, L. *et al*, *Collect. Czech. Chem. Commun.*, 1968, **33**, 3670 (*thermal props*)
Masse, R. *et al*, *J. Solid State Chem.*, 1980, **32**, 177 (*synth, cryst struct*)
Merck Index, 11th Ed., 1989, No. 8461.

IC-000043

$AgI_2O_{12}^{7\ominus}$
Bis[orthoperiodato(5−)-*O,O'*]argentate(*III*)(7−)
[12291-25-7]



M 553.6 (ion)
Square planar at Ag. Used in analytical work.
Penta-Na salt, di-H compd.: [103194-03-2].
$AgH_2I_2Na_5O_{12}$ M 670.6
Orange red cryst. (cold H_2O).
Ambrose, J. *et al*, *J. Electroanal. Chem. Interfacial Electrochem.*, 1973, **42**, 146 (*synth, props*)
Balikungeri, A. *et al*, *Inorg. Chim. Acta*, 1977, **22**, 7; 1978, **29**, 141 (*synth, ir, anal, uv-vis*)

IC-000044

$AgInS_2$
Indium silver sulfide ($InAgS_2$), 9Cl
[12002-75-4]
$AgInS_2$
M 286.8
Chalcopyrite-type struct. There is a high-temp. phase with a distorted wurtzite struct. and a high-pressure phase with the NaCl struct. Prepd. from Ag_2S + In_2S_3 or from the elements. Grey-black cryst. Semiconductor. Mp 880°.
Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1953, **271**, 153 (*synth*)
Range, K.J. *et al*, *Z. Naturforsch., B*, 1969, **24**, 1060; 1651 (*polymorphism*)
Roth, R.S. *et al*, *Mater. Res. Bull.*, 1973, **8**, 333 (*cryst struct, polymorph*)
Spiess, H.W. *et al*, *Phys. Status Solidi B*, 1974, **62**, 183 (*In-115 nmr*)

IC-000045

$AgInSe_2$
Indium silver selenide ($InAgSe_2$), 9Cl
[12002-76-5]
$AgInSe_2$
M 380.6
Chalcopyrite-type struct. High-pressure polymorphs are known. Prepd. from Ag_2Se + In_2Se_3 or from the elements. Grey-black cryst. Semiconductor. Mp 787°.
Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1953, **271**, 153 (*synth*)
Lerner, L.S. *et al*, *J. Phys. Chem. Solids*, 1966, **27**, 1 (*synth, props*)
Range, K.J. *et al*, *Z. Naturforsch., B*, 1968, **23**, 1262; 1969, **24**, 1063 (*synth, phase transition*)
Tell, B. *et al*, *J. Appl. Phys.*, 1974, **45**, 5367 (*electrical props*)
Spiess, H.W. *et al*, *Phys. Status Solidi B*, 1974, **62**, 183 (*In-115 nmr*)

IC-000046

$AgIn_5Te_8$
Indium silver telluride ($InAgTe_2$), 9Cl
[12002-77-6]
$AgInTe_2$
M 465.1
Chalcopyrite struct. A high-pressure phase with the NaCl struct. and a phase with the zinc-blende struct. are also known. Prepd. from Ag_2Te + In_2Te_3 or from the elements. Grey-black cryst. Semiconductor. Mp 692°.
Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1953, **271**, 153 (*synth*)
Range, K.J. *et al*, *Z. Naturforsch., B*, 1968, **23**, 1008; 1969, **24**, 813; 1970, **25**, 1187 (*polymorphs*)

IC-000047

AgLa
Lanthanum silver (1:1)
Silver lanthanum (AgLa)
[12041-03-1]
AgLa
M 246.7
Alloy with CsCl struct. Superconductor. Metal. Mp 835°
Dwight, A.E., *U.S. At. Energy Comm., ANL-6989*, 1959, 34 (*struct*)
Chao, C.-C. *et al*, *J. Appl. Phys.*, 1963, **34**, 1971 (*struct*)
Chao, C.-C. *et al*, *J. Phys. Chem. Solids*, 1966, **27**, 1551 (*supercond*)
Hill, R.W. *et al*, *J. Phys. C*, 1985, **16**, 2871 (*heat capacity*)

Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)
Bauer, E. *et al*, *Z. Phys. B: Condens. Matter*, 1986, **64**, 151 (*electronic struct*)

IC-000048

[AgLi]

Silver-lithium system
Lithium-silver system
Two alloy phases descr. here.

Silver lithium *(1:1)* [12002-78-7]
AgLi M 114.8
Has CsCl-type struct.

Silver lithium *(4:9)* [37189-86-9]
Ag_4Li_9 M 493.9
Struct. similar to γ-brass.

Zintl, E. *et al*, *Z. Phys. Chem., Abt. B*, 1933, **20**, 245 (*AgLi, struct*)
Freeth, W.E. *et al*, *J. Inst. Met.*, 1953, **82**, 569 (Ag_4Li_9, *struct*)
Norris, C.A. *et al*, *Phys. Status Solidi A*, 1970, **2**, 381 (*electronic struct, AgLi*)
Arnberg, L. *et al*, *Acta Chem. Scand.*, 1972, **26**, 1748 (Ag_4Li_9, *struct*)
Neubert, A. *et al*, *J. Chem. Soc., Faraday Trans. 1*, 1974, **70**, 2219 (*ms, AgLi*)
Gelatt, C.D. *et al*, *Phys. Rev. B: Condens. Matter*, 1983, **27**, 2005 (*theory, AgLi*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

[AgMg]

IC-000049

Silver-magnesium system
Magnesium-silver system

Silver magnesium *(1:1)* [12002-79-8]
β'-Silver magnesium
AgMg M 132.1
CsCl struct.

Silver magnesium *(1:3)* [12041-07-5]
ε-Silver-magnesium
$AgMg_3$ M 180.7
Hexagonal struct. Metallic.

Ageew, N.V. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1937, 289 (*struct, $AgMg_3$*)
Hume-Rothery, W. *et al*, *J. Inst. Met.*, 1940, **66**, 191 (*struct, AgMg*)
Letner, H.R. *et al*, *J. Appl. Phys.*, 1947, **18**, 833 (*struct, AgMg*)
Steeb, S. *et al*, *Z. Metallk.*, 1966, **57**, 374 (*struct, $AgMg_3$*)
Gavert, R.B. *et al*, *Trans. Metall. Soc. AIME*, 1967, **239**, 130 (*phys props, AgMg*)
Schmidt, P.C. *et al*, *Z. Metallk.*, 1976, **67**, 250 (*theory, AgMg*)
Kasai, P.H. *et al*, *J. Phys. Chem.*, 1978, **82**, 1554 (*esr, AgMg*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

$AgNO_2$

IC-000050

Silver(*I*) nitrite ($AgNO_2$)
Argentous nitrite
[7783-99-5]

$AgNO_2$

M 153.8
Has orthorhombic struct. similar to $NaNO_2$. Used to prepare standard $NaNO_2$ soln. for water anal.; reagent for prepn. of aliphatic nitro-compds. Commercially available. Non-hygroscopic pale yellow needles. Mod. sol. boiling H_2O; insol. alcohols. Dec. at 140°. Dec. by dil. acids or by prolonged boiling in H_2O. ΔH_f° −24.86 kJ mol^{-1}, ΔG_f° 11.11 kJ mol^{-1}.

Hess, H., *Ann. Physik. Chem.*, 1828, **12**, 257 (*synth*)
Prasad, M. *et al*, *Proc. Indian. Acad. Sci., Sect. A*, 1950, **31**, 389 (*magnetism*)
Haworth, F.E., *J. Appl. Phys.*, 1951, **22**, 606 (*thermal props*)
Plummer, C.W. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2720 (*synth, use*)
Eberhardt, W.H., *J. Chem. Phys.*, 1954, **22**, 1462 (*uv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1011 (*use*)
Patil, K.C. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 155 (*ir*)
Ohba, S. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 1911 (*cryst struct*)
Merck Index, 11th Ed., 1989, No. 8466.

$AgNO_3$

IC-000051

Silver nitrate ($AgNO_3$)
[7761-88-8]

$AgNO_3$

M 169.8
Phase transition between low temp. orthorhombic form and rhombohedral form takes place at 159°. Topical antiinfective agent. Used in photography; manuf. of mirrors; silver plating; colouring porcelain; v. important analytical reagent. Commercially available. Colourless, odourless, transparent, large cryst. or small white cryst. Not photosensitive when pure. Sol. H_2O, EtOH; mod. sol. Me_2CO; readily sol. aq. NH_3. Mp 212°. Presence of trace amounts of organic material promotes photoreduction. Dec. at 440° into metallic silver, nitrogen, oxygen and nitrogen oxides. ΔH_f° −123.6 kJ mol^{-1}, ΔG_f° −32.3 kJ mol^{-1}.

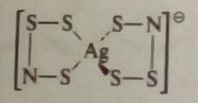
▷ Poisonous, caustic and irritant. VW4725000.

U.S. Pat., 2 581 518, (1948); *CA*, **47**, 6619f (*synth*)
U.S. Pat., 2 581 519, (1948); *CA*, **47**, 6619g (*synth*)
Rhodes, E. *et al*, *Proc. R. Soc. London*, 1959, **251**, 156 (*phase transition*)
Niggli, A., *Z. Kristallogr.*, 1959, **111**, 269 (*cryst struct*)
Mosley, W.C. *et al*, *J. Chem. Phys.*, 1965, **43**, 1207 (*esr*)
Meyer, P., *Acta Crystallogr., Sect. B*, 1976, **32**, 1143; 1982, **38**, 2543 (*cryst structs*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **21**, 19 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 5321.
Merck Index, 11th Ed., 1989, No. 8464.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3031.

$AgN_2S_6^{\ominus}$

IC-000052

[Bis(dithioperoxy)thionitrito]argentate(1−), 11Cl



M 328.2 (ion)
Struct. analogous to [Bis(dithioperoxy)thionitrito] cuprate(1−), IC-017909.

Bis(triphenylphosphine)iminium(1+) salt: [81519-34-8]. Synth. from $AgNO_3$ and $(Ph_3P)_2N^{\oplus}S_3N^{\ominus}$ in MeCN. Orange cryst. Sol. MeCN.

Bojes, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1981, 1171 (*synth, uv-vis*)

AgO

IC-000053

Silver(*I,III*) oxide (AgO)
Argentic oxide. Silver peroxide. Silver suboxide. Dirasil
[1301-96-8]

$Ag^{I}Ag^{III}O_2$

M 123.8
Mixed oxidation state oxide with 4-coordinate Ag(*III*) and 2-coordinate (linear) Ag(*I*). Used in manuf. of silver oxide-zinc alkali batteries. Commercially available. Charcoal grey powder. Malleable. Insol. H_2O; sol. alkalis, $[NH_4]OH$ (with dec.). Dec. >100° into silver and oxygen; semiconductor; diamagnetic; strong oxidising agent.

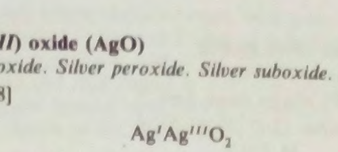
▷ Avoid contact with skin, organic matter, strong ammonia and alkalis.

Watson, E.R., *J. Chem. Soc.*, 1906, 578 (*synth*)
Neiding, A.B., *Dokl. Akad. Nauk SSSR*, 1951, **78**, 713 (*magnetism*)
Inorg. Synth., 1953, **4**, 12 (*synth*)
Graff, W.S. *et al*, *J. Electrochem. Soc.*, 1958, **105**, 446 (*synth*)
McMillan, J.A., *J. Inorg. Nucl. Chem.*, 1960, **13**, 28 (*theory, conductivity, cryst struct*)
Scatturin, V. *et al*, *Ric. Sci.*, 1960, **30**, 1034 (*nd*)
McMillan, J.A., *Chem. Rev.*, 1962, **62**, 65 (*rev*)
Dirske, T.P., *J. Electrochem. Soc.*, 1964, **108**, 813 (*use*)
Chem. Eng. News, 1969, **47**, 32 (*synth, single cryst*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 998 (*synth*)
Merck Index, 11th Ed., 1989, No. 8469.

$AgO_{12}Te_2^{9\ominus}$

IC-000054

Bis[orthotellurato(6−)-*O,O'*]argentate(*III*)(9−)
Bis[hexaoxotellurato(6−)]argentate(III)(9−).
Diorthotelluratoargentate(III)(9−)
[12291-30-4]



M 555.0 (ion)
Square planar at Ag. Oxidising agent e.g. for aliphatic amines; has applications in analysis, via its oxidative ability.

Penta-K salt, tetra-H compd.: [12510-72-4].
$AgH_4K_5O_{12}Te_2$ M 754.5
Orange cryst. (cold H_2O).
[67606-05-7]

Balikungeri, J. *et al*, *Inorg. Chim. Acta*, 1977, **22**, 7; 1978, **29**, 141 (*synth, ir, anal, uv-vis*)
Ravi Prasad, T. *et al*, *Indian J. Chem., Sect. A*, 1982, **21**, 169 (*use as oxidant, kinetics*)

[AgPb]

IC-000055

Silver-lead system
Lead-silver system

Silver lead *(4:1)*
Ag_4Pb M 638.6

Heidenreich, R.D., *Acta Metall.*, 1955, **3**, 79 (*struct*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

$AgPbS_3Sb$

IC-000056

Freieslebenite
Lead silver antimonide sulfide ($PbAgSbS_3$)
[29191-46-6]

$PbAgSbS_3$

M 533.0
Mineral, occurs in USSR, Peru, Czechoslovakia. Lead grey to silver white metallic cryst.

Navaki, W. *et al*, *Minerogenezis*, 1974, 119 (*cryst struct*)
Friedrich, M., *Bel. Geowiss. Abh., Reihe A*, 1983, **46**, 109.
Megarskaja, L. *et al*, *Acta Mont.*, 1984, **68**, 237; 1985, **70**, 21; *CA*, **105**, 176025n (*synth*)

[AgPt]

IC-000057

Platinum-silver system
Silver-platinum system
Alloy; two phases descr. here.

Platinum silver *(3:1)* [37189-85-8]
α''-Platinum-silver
$AgPt_3$ M 693.1
Has Cu_3Au-type struct. Metallic.

Platinum silver *(1:3)*
Ag_3Pt M 518.6
Has Cu_3Au-type struct. Metallic.

Schneider, A. *et al*, *Z. Elektrochem.*, 1943, **49**, 72 ($AgPt_3$, *struct*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

[AgSb]

IC-000058

Silver-antimony system
Antimony silver

Silver antimony *(7:1)*
ζ-Silver-antimony
Ag_7Sb M 876.8
From Ag_3Sb to Ag_7Sb deformed similar phases are formed. Approx. A3 (Mg-type) struct. – hcp.

Silver antimony *(3:1)* [14176-81-9]
ε-Silver-antimony
Ag_3Sb M 445.3
β'-$TiCu_3$ type struct.

Weibke, F. *et al*, *Z. Elektrochem.*, 1940, **46**, 52 (Ag_3Sb, *struct*)
Burkhardt, W. *et al*, *Z. Metallk.*, 1959, **50**, 442 (Ag_3Sb, *struct*)
King, H.W. *et al*, *Philos. Mag.*, 1961, **6**, 669 (Ag_3Sb, *struct*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

[AgSn]

IC-000059

Silver-tin system
Tin-silver system
Two phases reported here.

Silver tin *(5:1)*
ζ-Silver-tin
Ag_5Sn M 658.0
Mg-type struct.-hcp.

Silver tin *(3:1)* [12041-38-2]
γ-Silver-tin
Ag_3Sn M 442.3
β'-$TiCu_3$ type struct.

Westgren, A., *Z. Metallk.*, 1926, **18**, 279 (Ag_5Sn, *struct*)
Nial, O. *et al*, *Z. Phys. Chem., Abt. B*, 1931, **14**, 83 (Ag_5Sn, Ag_3Sn, *struct*)
Michel, P., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1952, **235**, 377 (Ag_3Sn, *struct*)
King, H.W. *et al*, *Philos. Mag.*, 1961, **6**, 669 (Ag_3Sn, *struct*)

Pinsbarn, C.W. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 371 (*Ag_5Sn, struct*)
Gonser, H.E. *et al*, *J. Biomed. Mater. Res.*, 1975, **9**, 207 (*Ag_5Sn, magn*)
Silva, J. *et al*, *J. Mater. Sci.*, 1978, **13**, 836 (*Ag_5Sn, mössbauer*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

IC-000060

[AgTh]

Thorium-silver system
Silver-thorium system

Thorium silver *(2:1)* [12785-36-3]
$AgTh_2$ M 571.9
$CuAl_2$-type struct. Superconducting at 2.26K.

Meaves, J.R., *J. Inst. Met.*, 1955, **84**, 91 (*struct*)
Matthias, B.T. *et al*, *Phys. Chem. Solids*, 1961, **19**, 130 (*supercond*)
Hawiga, E.E. *et al*, *J. Less-Common Met.*, 1972, **27**, 281 (*supercond*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

IC-000061

AgTi

Titanium silver (1:1)
Silver titanium (AgTi)
[12002-89-0]

$AgTi$

M 155.7
Alloy with CuAu-type struct. Metallic.

McQuillan, M.K., *J. Inst. Met.*, 1959, **88**, 235 (*struct*)
Schuberl, K., *Z. Metallk.*, 1965, **56**, 197 (*struct*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

IC-000062

[AgZn]

Silver-zinc system
Zinc-silver system
Several phases known.

Silver zinc *(1:1)* [12041-17-7]
AgZn M 173.2
Metallic.
β-form: High temp. struct. A2 (W-type) struct. cubic close-packed.
β'-form: Medium temp. struct. CsCl-type struct.
ζ-form: Struct. obt. below 260°. Bb struct. type.

Silver zinc *(5:8)* [86703-30-8]
γ-Silver-zinc
Ag_5Zn_8 M 1062.4
γ-brass struct.

Silver zinc *(1:3)* [52037-01-1]
ε-Silver-zinc
$AgZn_3$ M 304.0
Has hcp struct. which resembles that of Mg.

Weerts, J., *Z. Metallk.*, 1932, **24**, 265 (*AgZn, struct*)
Owen, E.A. *et al*, *Proc. R. Soc. London, A*, 1933, **140**, 344; 1938, **50**, 389 (*struct, $AgZn_3$, AgZn*)
Owen, E.A. *et al*, *J. Inst. Met.*, 1935, **57**, 297 (*$AgZn_3$, struct*)
Edmunds, I.G. *et al*, *Acta Crystallogr.*, 1951, **4**, 417 (*AgZn, struct*)
Hume-Rothery, W. *et al*, *J. Inst. Met.*, 1951, **80**, 609 (*Ag_5Zn_8, struct*)
Marsh, R.E., *Acta Crystallogr.*, 1954, **7**, 379 (*Ag_5Zn_8, struct*)
Abriata, J.P. *et al*, *Scr. Metall.*, 1968, **2**, 41 (*AgZn, struct*)
Kasai, P.H. *et al*, *J. Phys. Chem.*, 1978, **82**, 1554 (*AgZn, esr*)
Iwasaki, H. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1762 (*Ag_5Zn_8, struct*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

IC-000063

[AgZr]

Zirconium-silver system
Silver-zirconium system
Alloy; two phases descr. here.

Zirconium silver *(2:1)* [37381-03-6]
$AgZr_2$ M 290.3
Has $MoSi_2$-type struct. Metallic.

Zirconium silver *(1:1)* [37381-02-5]
AgZr M 199.0
Has CuAu-type struct. Metallic.

Raub, E. *et al*, *Z. Metallk.*, 1948, **39**, 172 (*AgZr, struct*)
Karlsson, N., *Acta Chem. Scand.*, 1952, **6**, 1424 (*AgZr, struct*)
Betterton, J.O. *et al*, *Trans. Am. Inst. Min., Metall. Pet. Eng.*, 1958, **212**, 470 (*phase diagram, struct*)
Nevitt, M.V. *et al*, *Trans. Am. Inst. Min., Metall. Pet. Eng.*, 1962, **224**, 195 (*$AgZr_2$, struct*)
Brewer, L. *et al*, *Metall. Trans.*, 1973, **4**, 83 (*$AgZr_2$, thermodyn*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

IC-000064

Ag_2BaS_4Sn

Barium disilver thiostannate
Barium silver tin sulfide (BaAg₂SnS₄). Barium silver tetrathioxostannate, 9CI
[61036-11-1]

Ag_2BaSnS_4

M 600.0
Orthorhombic cryst.

Teske, C.L. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **426**, 281 (*synth, cryst struct*)

IC-000065

Ag_2CrO_4

Silver(*I*) chromate(*VI*) (Ag_2CrO_4)
[7784-01-2]

Ag_2CrO_4

M 331.7
Struct. comprises an interlocking network where Ag ions are coordinated by chromate group oxygens. Tetragonal bipyramidal and distorted tetrahedral coordinations exist. Catalyst for formation of aldol from alcohol; formed at end point of Mohr titration of halides. Commercially available. Dark brownish-red cryst. powder. Spar. sol. H_2O. Sol. HNO_3, NH_3. Mp 665°. Diamagnetic.

Baxter, P. *et al*, *J. Am. Chem. Soc.*, 1909, **31**, 541 (*anal*)
Hess, K. *et al*, *Z. Phys. Chem.*, 1932, **A162**, 153 (*soly*)
Norman, C.C.L., *J. Chin. Chem. Soc. (Peking)*, 1938, **6**, 51 (*electrochem*)
Szmal, Z., *Wiad. Chem.*, 1954, **8**, 241; *CA*, **49**, 7445h (*tga*)
Symons, M.C.R. *et al*, *J. Chem. Soc.*, 1962, 3503 (*uv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1005 (*use*)
Hackert, M.L. *et al*, *J. Solid State Chem.*, 1971, **3**, 364 (*cryst struct, synth*)
Merck Index, 11th Ed., 1989, No. 8456.

IC-000066

Ag_2F

Silver fluoride (Ag_2F)
Silver subfluoride. Disilver fluoride
[1302-01-8]

Ag_2F

M 234.7
Struct. comprises successive layers of Ag, Ag and F with Ag—Ag 299.6 and 281.4 pm and Ag—F 245.1 pm.

Hexagonal, bronze-coloured cryst. with green lustre. Good electrical conductor. Turns greyish-black on prolonged exp. to air. ΔH_f° −211.7 kJ mol^{-1}. Thermal dec. to Ag and AgF begins at 100° and is complete by 200°. Instant hydrol. with H_2O to precipitate silver powder. Stable to EtOH and light.

Hettich, A., *Z. Anorg. Allg. Chem.*, 1927, **167**, 67 (*synth*)
Inorg. Synth., 1957, **5**, 18 (*synth*)
Trzebiatowski, W. *et al*, *Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 183 (*conductivity*)
Wagener, K., *Z. Phys. Chem.*, 1960, **25**, 135 (*thermodyn*)
Argay, G. *et al*, *Acta Chim. Acad. Sci. Hung.*, 1966, **49**, 329 (*cryst struct*)
Merck Index, 11th Ed., 1989, No. 8479.

IC-000067

Ag_2FeS_4Sn

Iron silver tin sulfide ($FeAg_2SnS_4$)
[12376-96-4]

Ag_2FeSnS_4

M 518.5
Mineral-form [37342-34-0]
Hocartite
Occurs assoc. with wurtzite and sphalerite. Brown-grey; granular.

Caye, R.C. *et al*, *Bull. Soc. Fr. Minéral. Cristallogr.*, 1968, **91**, 383 (*phys prop, struct*)
Caye, R.C. *et al*, *Am. Mineral.*, 1969, **54**, 573.
Povarennykh, A.S., *Mineral. Zh.*, 1981, **3**, 16 (*ir*)

IC-000068

$Ag_2Ge_2O_5$

Germanium silver oxide ($Ag_2Ge_2O_5$)
Silver germanate
[12645-39-5]

$Ag_2Ge_2O_5$ or $Ag_2O.2GeO_2$

M 440.9
Typical formula of a series of silver germanate glasses. Synth. from Ag_2O and GeO_2 in Pt crucible at 1470°. Colourless, through light yellow to deep red glass depending on % Ag_2O.

Riebling, E.F., *J. Chem. Phys.*, 1971, **55**, 804, 3921 (*synth*)
Riebling, E.F., *J. Mater. Sci.*, 1972, **7**, 40 (*struct, ir*)

IC-000069

Ag_2HgI_4

Silver(*I*) tetraiodomercurate(*II*) ($Ag_2(HgI_4)$)
Mercury silver iodide ($HgAg_2I_4$)
[7784-03-4]

$Ag_2(HgI_4)$

M 923.9
The r.t. β-form struct. is tetragonal with chalcopyrite type of cation ordering and considerable distortion of the anion cubic close packing. Transforms to α-form above 50°, in which the silver ions are highly mobile. Thermal sensor, becomes blood red at 40-50° and yellow again on cooling. Deep yellow thermochromic powder. Insol. H_2O, dil. acids; sol. solns. of alkali iodides or cyanides. Mp 652°. ΔH_f° −716.1 kJ mol^{-1}.

Lietzke, M.H. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1877 (*sol*)
Kroge-Moe, J., *Sel. Top. High Temp. Chem.*, 1966, 79; *CA*, **65**, 11455b (*conductivity*)
Geller, S., *Fast Ion Transp. Solids*, Solid State Batteries Devices, Proc. NATO Adv. Study Inst., (Van Gool, W. Ed.), North Holland, Amsterdam, 1973, 607 (*conductivity*)
Browall, K.W. *et al*, *J. Solid State Chem.*, 1974, **10**, 20 (*cryst struct, β-form, synth*)
Kasper, J.S. *et al*, *J. Solid State Chem.*, 1975, **13**, 49 (*cryst struct, α-form*)
Iwe, H.R.C. *et al*, *Inorg. Chem.*, 1987, **26**, 1387 (*synth, str, thermal props*)
Merck Index, 11th Ed., 1989, No. 8482.

IC-000070

Ag_2MoO_4

Silver molybdate(*VI*) (Ag_2MoO_4)
Molybdenum silver oxide ($MoAg_2O_4$). Disilver molybdate
[13765-74-7]

Ag_2MoO_4

M 375.6
Contains the tetrahedral $[MoO_4]^{2\ominus}$ ion. Spinel type lattice. Synth. by combining aq. solns. of sodium or ammonium molybdate and a sol. silver salt or by fusing $AgNO_3$ and MoO_3 at 500-600°. White solid; yellow solid (after fusion), or cubic cryst. Readily melts to yellow liq. Insol. H_2O; sol. HNO_3. Mp 483°.

Wyckoff, R.W.G., *J. Am. Chem. Soc.*, 1922, **44**, 1994 (*struct*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1931, **11**, 559 (*rev, bibl*)
Donohue, J. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 222 (*struct*)

IC-000071

Ag_2O

Silver(*I*) oxide (Ag_2O)
Argentous oxide
[20667-12-3]

Ag_2O

M 231.7
Struct. consists of fcc arrangement of silver ions interpenetrated by a bcc arrangement of oxygen ions. Each oxygen tetrahedrally coordinated by silver. Isostructural with Cu_2O. Catalyst; used in the purif. of drinking water; in the glass industry (polishing, colouring glass yellow). Commercially available. Brownish-black, heavy, odourless powder. Light sensitive. Insol. alcohols. V. spar. sol. H_2O. Freely sol. dil. HNO_3, NH_3. Begins to dec. at 200° and at 250-300° dec. is rapid. When moist, absorbs CO_2. ΔH_f° −30.7 kJ mol^{-1}.

▷ VW4900000.

Madsen, C., *Z. Anorg. Allg. Chem.*, 1913, **79**, 197 (*synth*)
Davey, W.P., *Phys. Rev.*, 1922, **19**, 248 (*cryst struct*)
Niggli, P., *Z. Kristallogr.*, 1922, **57**, 253 (*cryst struct*)
Riley, H.L. *et al*, *J. Chem. Soc.*, 1926, 2510 (*synth, props*)
Hsieh, S.L. *et al*, *CA*, 1960, **54**, 5312c (*synth*)
McDevitt, N.T. *et al*, *Spectrochim. Acta*, 1964, **20**, 799 (*ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 998 (*synth*)
Merck Index, 11th Ed., 1989, No. 8468.

IC-000072

Ag_2O_2Pb

Lead silver oxide ($PbAg_2O_2$)
Silver plumbite
[12249-87-5]

Ag_2PbO_2

M 454.9
Predominantly covalent bonding. Pb is coordinated by 4 O (*cf* PbO). Yellow-brown or brown prismatic cryst. with metallic lustre, or olive-coloured powder. Insol. H_2O, aq. NH_3; sol. dil. HNO_3, conc. acid. On heating to ~140-150°, becomes grey-black. Dec. on melting.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1927, **7**, 668 (*rev*)

Bowman, A. *et al*, *Acta Chem. Scand.*, 1950, **4**, 813 (*synth, cryst struct*)
Dickens, B., *J. Inorg. Nucl. Chem.*, 1966, **28**, 2793 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst No. 61, 1974, **B4**, 252 (*bibl*)

IC-000073

Ag_2O_3S
Silver(1+) sulfite (Ag_2SO_3)
[13465-98-0]

Ag_2SO_3

M 295.8
Prepd. from Na_2SO_3 or SO_2 + $AgNO_3$ soln. Commercially available. White cryst. Unstable to light and heat. Spar. sol. H_2O.

Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, **2**, 1043 (*synth*)
Larsson, L.O., *Acta Chem. Scand.*, 1969, **23**, 2261 (*cryst struct*)
Nyberg, B. *et al*, *Acta Chem. Scand.*, 1973, **27**, 63 (*ir*)

IC-000074

Ag_2O_3Se
Silver(*I*) selenite (Ag_2SeO_3)
[7784-05-6]

Ag_2SeO_3

M 342.6
Needles. Spar. sol. cold H_2O; sol. hot H_2O, HNO_3. Mp 530°. ΔH_f° −367 kJ mol^{-1}. Dec. >530° to Ag, SeO_2, O_2.

Senderens, J.B., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1887, **104**, 174 (*synth*)
Prasad, M. *et al*, *Proc. - Indian Acad. Sci., Sect. A*, 1950, **31**, 389 (*magnetism*)
Rocchiccioli, C., *Ann. Chim.*, 1960, **5**, 999 (*ir*)
Buketov, E.A. *et al*, *Zh. Neorg. Khim.*, 1964, **9**, 2701 (*thermal props*)
Bakeeva, S.S. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 16.
Merck Index, 11th Ed., 1989, No. 8478.

IC-000075

Ag_2O_3Si
Silver silicate ($Ag_4(Si_2O_6)$)
Silver(I) metasilicate
[16625-98-2]

$Ag_4[Si_2O_6]$

M 291.8
Single chain silicate ($2SiO_4$ tetrahedra per chain). Prepd. by fusion of Na_2SiO_3 or Li_2SiO_3 with excess $AgNO_3$ at 300°. Yellow cryst. Dec. at 400°. Stable to H_2O.

Thilo, E. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **295**, 247 (*synth, struct*)
Gessner, W., *Wiss. Z. Hochsch. Archit. Bauwes. Weimar*, 1968, **15**, 185 (*synth*)
Völlenkle, H. *et al*, *Z. Kristallogr.*, 1981, **154**, 77.

IC-000076

Ag_2O_4S
Silver(*I*) sulfate (Ag_2SO_4)
[10294-26-5]

Ag_2SO_4

M 311.8
The r.t. β-form is rhomohedral and transforms to the hexagonal α-form above 425°. Commercially available. Cryst. or powder which darkens on exp. to light. Spar. sol. H_2O; sol. HNO_3, NH_3, conc. H_2SO_4. Mp 657°. Dec. at 1085°.

Hsieh, S.L. *et al*, *CA*, **54**, 5312c (*synth*)

Richards, T.W. *et al*, *Z. Anorg. Allg. Chem.*, 1907, **55**, 72 (*synth*)
Herrmann, K. *et al*, *Z. Kristallogr.*, 1931, **80**, 402 (*cryst struct, ß-form*)
Hsq, M.I. *et al*, *Nature* (*London*), 1936, **137**, 907 (*str*)
Prasad, M. *et al*, *Proc. Indian. Acad. Sci., Sect. A*, 1950, **31**, 389 (*magnetism*)
Fischmeister, H.F., *Z. Phys. A.*, 1956, **7**, 91 (*cryst struct, α-form*)
Lietzke, M.H. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1877 (*solv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1015 (*use*)
Baron, E.J. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 288 (*ir*)
Merck Index, 11th Ed., 1989, No. 8480.

IC-000077

Ag_2O_4Se
Silver(*I*) selenate (Ag_2SeO_4)
[7784-07-8]

Ag_2SeO_4

M 358.6
Several cryst. modifications are known; r.t. form is isostructural with Na_2SO_4. Orthorhombic cryst. ΔH_t° −422.1 kJ mol^{-1}; Phase transitions occur at 425° and 537°.

Gerbach, R.W. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 1054 (*synth*)
Selivanova, N.M. *et al*, *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1959, **33**, 430 (*synth*)
Ladd, W.H.L. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **21**, 216 (*cryst struct*)
Sathianandan, K. *et al*, *Spectrochim. Acta*, 1964, **20**, 957 (*ir*)
Pistorius, C.W.F.T. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **372**, 263 (*phase props, dta, powder struct*)
Merck Index, 11th Ed., 1989, No. 8476.

IC-000078

$Ag_2O_5Si_2$
Silver silicate ($Ag_2Si_2O_5$)
Silver disilicate
[61204-22-6]

$Ag_2Si_2O_5$

M 351.9
A single-layer silicate. Synth. by fusion of $Na_2Si_2O_5$ with $AgNO_3$ at 300°. Yellow cryst.

Liebau, F., *Acta Crystallogr.*, 1961, **14**, 537 (*cryst struct*)
Thilo, E. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **295**, 247 (*synth, struct*)

IC-000079

Ag_2S
Silver(*I*) sulfide (Ag_2S)
Argentous sulfide
[21548-73-2]

Ag_2S

M 247.8
Monoclinic at r.t., transforming to bcc at 117° and to fcc at 593°. β-Ag_2S is an electronic as well as a cation-disordered fast ion conductor between 177° and 593°. Used in ceramics. Commercially available. Greyish-black, heavy powder. Insol. H_2O; sol. HNO_3, solns. of alkali cyanides. ΔH_f° −31.9 kJ mol^{-1}. Dec. with loss of sulfur >200°.

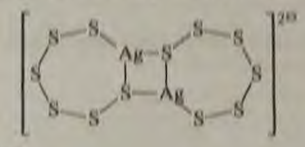
Mineral-form
Argentite
Occurs. e.g. in Western USA; major ore in Mexico; also found in some European countries. Commonly assoc. with Ag and galena. Lead-grey to blackish lead-grey opaque cryst.

Hönigschmid, O. *et al*, *Z. Anorg. Allg. Chem.*, 1931, **195**, 207 (*synth*)

Kroge-Moe, J., *Sel. Top. High Temp. Chem.*, 1966, 79; *CA*, **65**, 114556 (*phase props*)
Okazaki, H. *et al*, *J. Phys. Soc. Jpn.*, 1967, **23**, 355 (*conductivity*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 999 (*synth*)
Cava, R.J. *et al*, *J. Solid State Chem.*, 1980, **31**, 69 (*cryst struct*)
Merck Index, 11th Ed., 1989, No. 8481.

IC-000080

$Ag_5S_{15}^{3\ominus}$
Bis[μ-(hexathio-S^1:S^1,S^6)]diargentate(2−), 11Cl
Bis(μ-hexasulfido-S,S:S')diargentate(1)(2−)



M 600.5 (ion)
Bis-Ph_4P salt: [94629-50-2].
Orange cryst.

Müller, A. *et al*, *Inorg. Chim. Acta*, 1984, **90**, L69 (*synth, cryst struct, raman*)

IC-000081

Ag_2Se
Silver(*I*) selenide (Ag_2Se)
Disilver selendide
[1302-09-6]

Ag_2Se

M 294.6
α-form has a bcc lattice of $Se^{2\ominus}$ with $Ag^{\oplus}$ randomly distributed in interstices. Transforms to β-form at 133°. Commercially available. Grey, hexagonal, microscopic needles. Insol. H_2O. Mp 880°. Diamagnetic. Forms metallic silver and selenium oxide when heated in oxygen. ΔH_f° −12.8 kJ mol^{-1}.

Mineral-form
Naumannite
Occurs in e.g. USA, Argentina, Germany assoc. with similar minerals. Greyish black opaque cubes; tarnishes→brown.

Pélabon, H., *Ann. Chim. Phys.*, 1902, **25**, 365 (*synth*)
Tubandt, C. *et al*, *Z. Elektrochem.*, 1933, **39**, 227 (*synth*)
Tubandt, C. *et al*, *Z. Phys. A.*, 1934, **24**, 22 (*conductivity*)
Sander, W., *Z. Phys.*, 1960, **159**, 456 (*ir*)
Wiegers, G.A., *Am. Mineral.*, 1971, **56**, 1882 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1000 (*synth*)
Merck Index, 11th Ed., 1989, No. 8477.

IC-000082

Ag_2Te
Silver telluride (Ag_2Te)
[12002-99-2]

Ag_2Te

M 343.3
Occurs in nature as the mineral Hessite. Prepd. by heating Ag in Te vapour. Commercially available. Black cryst. Polymorphic with transition temps. 149.5° and 800°. Insol. H_2O. Mp 955°.

[12002-98-1]

Hoenigschmid, O., *Z. Anorg. Allg. Chem.*, 1933, **214**, 281 (*synth*)
Frueh, A.J., *Z. Kristallogr.*, 1959, **112**, 44 (*cryst struct*)
Frueh, A.J., *Am. Mineral.*, 1961, **46**, 654 (*polymorphism*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1001 (*synth*)
Sakuma, T. *et al*, *J. Phys. Soc. Jpn.*, 1985, **54**, 3647 (*cryst struct*)

IC-000083

Ag_3AsO_4
Silver(*I*) arsenate ($Ag_3(AsO_4)$)
Trisilver(1+) arsenate, 9CI
[13510-44-6]

Ag_3AsO_4

M 462.5
Exhibits polymorphism. Low temp. and high temp. modifications (transition at 700-725°) are simple cubic and fcc respectively. Synth. from $AgNO_3$ + H_3AsO_4. Chocolate-brown solid. Mp 925-960°. Light sensitive.

Cordfunke, E.H.P. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1967, **86**, 93 (*synth, props*)
Joergensen, C.K. *et al*, *Kgl. Dan. Vidensk. Selsk. Mata.-Fys. Medd.*, 1972, **38** (*pe*)
Muck, A. *et al*, *Collect. Czech. Chem. Commun.*, 1980, **45**, 3262 (*ir*)
Namboodiri, P.N. *et al*, *Thermochim. Acta*, 1983, **60**, 55 (*synth, props, cryst struct*)

IC-000084

Ag_3AsS_3
Trisilver arsenotrithioite, 9CI
Silver trithioarsenite. Silver sulfoarsenite. Silver thioarsenite, 8CI. Silver arsenic sulfide (Ag_3AsS_3)
[15122-57-3]

Ag_3AsS_3

M 494.7
Consists of $(AsS_3)^{3\ominus}$ pyramids with each S attached to two $Ag^{\oplus}$ ions binding a given prism to its neighbours. At r.t. As—S 227.1 (mean), S—S 346, Ag—S 244.5 (mean) pm. Struct. retained down to transition at −244°. Below this temp. possesses monoclinic unit cell. Synth. from the elements. Used in acoustooptical devices for communication systems. Dark red solid. Mp 496°. Photoconductor and electric semiconductor possessing ferroelastic, piezoelectric props. Ferroelectric (Curie point −244°). Exhibits other phase transitions at −217 to −212°, and possibly −225°.

Mineral-form
Proustite. *Ruby silver. Light red silver ore*
Associated with Au and Ag ores. Found in Japan, Romania, Canada. Mp 484°.

Mineral-form [15122-59-5]
Xanthoconite. *Xanthokon. Xanthocone. Rittingerite*
Found in Czechoslovakia. Metastable.

Kovaleva, I.S. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 1512; *Inorg. Materials* (*Engl. Transl.*), 1971, **7**, 1340 (*synth, phase diagram*)
Golovei, M.I. *et al*, *Krist. Tech.*, 1971, **6**, 631 (*synth, bibl*)
Byer, H.H. *et al*, *Ferroelectrics*, 1973, **5**, 207 (*ir, raman*)
Taylor, W. *et al*, *Solid State Commun.*, 1980, **35**, 829 (*raman, props*)
Domashevskaya, E.P. *et al*, *Phys. Status Solidi B*, 1981, **106**, 429 (*pe*)
Rebane, L. *et al*, *Fiz. Tverd. Tela* (*Leningrad*), 1982, **24**, 2351; *Soviet Phys.: Solid State* (*Engl. Transl.*), 1982, **24**, 1335 (*raman*)
Gavrilova, N.D. *et al*, *Fiz. Tverd. Tela* (*Leningrad*), 1982, **24**, 3063; *Soviet Phys.: Solid State* (*Engl. Transl.*), 1982, **24**, 1735 (*optical, electrical props*)
O'Hara, C., *J. Phys. D*, 1982, **15**, 1289 (*props, uses*)
Bondar', A.V. *et al*, *Fiz. Tverd. Tela* (*Leningrad*), 1983, **25**, 2602; *Soviet Phys.: Solid State* (*Engl. Transl.*), 1983, **25**, 1497 (*ir*)
Ewen, P.J.S. *et al*, *J. Phys. C*, 1983, **16**, 6475 (*raman, struct*)
Nelmes, R.J. *et al*, *J. Phys. C*, 1984, **17**, L861 (*struct*)

Allen, S., *Phase Transitions*, 1985, **6**, 1 (*cryst struct*)
Sirs, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 302 (*haz*)

IC-000085

Ag_3O_4P
Silver phosphate ($Ag_3(PO_4)$)
Trisilver(1+) phosphate, 9CI. Silver orthophosphate
[7784-09-0]

Ag_3PO_4

M 418.5
Low (ordinary) temp. form is cubic. The regular PO_4 tetrahedra form a bcc lattice. The six Ag ions are disordered among 12 sites. Synth. from Ag_2O + $NH_4H_2PO_4$ at 400°; $AgNO_3$ aq. + Na_2HPO_4 or $(NH_4)_2HPO_4$ aq. Commercially available. Yellow cubes (NH_3 aq.). Mp 1012° (980-990°). Suspensions photochemically release O from H_2O more efficiently than AgCl in phosphate buffer. At 520° (505°) undergoes transition to high temp. form with fcc cubic lattice. V. sensitive to light, becoming red.

Gmelin Handbook Inorg. Chem., Syst. No. 6, 1974, **B4**, 7.
Sokolova, I.D. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1975, **221**, 1126; *Dokl. Phys. Chem.* (*Engl. Transl.*), 1975, **221**, 378 (*props*)
Dickinson, T. *et al*, *J. Solid State Chem.*, 1975, **13**, 237 (*pe*)
Masse, R. *et al*, *Z. Krisnallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1976, **144**, 76 (*cryst struct*)
Ng, H.N. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 898 (*synth, cryst struct*)
Newsam, J.M. *et al*, *Solid State Ionics*, 1980, **1**, 377; 1984, **14**, 81 (*nd. struct*)
Hirono, T. *et al*, *J. Appl. Phys.*, 1984, **55**, 781 (*synth, ac, struct, props*)
Prabhakar, S. *et al*, *Chem. Phys. Lett.*, 1987, **139**, 96 (*P-31 nmr*)

$Ag_3Pb_2S_5Sb_3$ IC-000086
Diaphorite
Lead silver antimonide sulfide ($Pb_2Ag_3Sb_3S_8$)
[12214-31-2]

$Ag_3Pb_2Sb_3S_8$

M 1359.7
Mineral found in USSR and in tin/silver deposit in USSR. Steel grey metallic cryst.

Andrievskii, A.I. *et al*, *Fiz. Elektron.* (*Lvov*), 1972, 6 (*synth*)
Megarskaja, L. *et al*, *Acta Mont.*, 1984, **68**, 237; 1985, **70**, 21; *CA*, **105**, 176025n (*synth*)

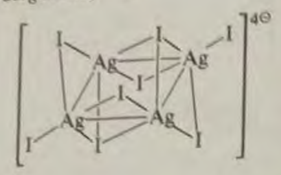
Ag_3S_3Sb IC-000087
Antimony silver sulfide ($SbAg_3S_3$)
[15983-65-0]

Ag_3SbS_3

M 541.5
Synth. from Ag_2S + Sb_2S_3; or from AgCl + Sb_2S_3 at 300°, or Ag + Sb + S at <650°. Deep red solid or purplish-red cryst. with metallic lustre. Mp 473°. Photosensitive ferroelectric semiconductor. Exhibits high ir transparency. Exhibits a phase transition at −263°.
Mineral-form [15123-77-0]
Pyrargyrite. *Ruby silver. Dark red silver ore*
Associated with other Ag and Au ores in Japan and USSR. Also found in USA (Nevada) and Canada (Manitoba) as well as in East European countries. Of potential use in acoustooptical devices.

Dovgii, Ya.O. *et al*, *Kristallografiya*, 1971, **16**, 1043; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1971, **16**, 912 (*ir*)
Holovey, M.I. *et al*, *Krist. Tech.*, 1973, **8**, 453 (*synth, ac, props*)
Stevens, J.G. *et al*, *Inorg. Nucl. Chem. Lett.*, 1977, **13**, 595 (*mössbauer*)
Sugaki, A. *et al*, *Sci. Rep. Tohoku Univ., Ser. 3*, 1978, **14**, 53 (*synth*)
Bondar, A.V. *et al*, *J. Mol. Struct.*, 1982, **83**, 85 (*nqr*)
Baisa, D.F. *et al*, *J. Mol. Struct.*, 1982, **83**, 387 (*nqr*)
Ewen, P.J.S. *et al*, *J. Phys. C*, 1983, **16**, 6475 (*synth, raman*)
Brovina, S.L. *et al*, *Ferroelectrics*, 1987, **83**, 119.

$Ag_4I_8^{4\ominus}$ IC-000088
Di-μ_3-iodotetra-μ-iododiiodotetraargentate(4−)
Octaiodotetraorgentate(4−)



M 1446.7 (ion)
Bis(6,9-diazoniadispiro[5.2.5.3]heptadecane)(2+) salt:
[106207-62-9].
Cryst.

Estienne, J., *Acta Crystallogr., Sect. C*, 1986, **42**, 1512 (*synth, cryst struct*)

$Ag_4P_2S_7$ IC-000089
Tetrasilver(1+) thiodiphosphate, 9CI
Tetrasilver heptathiopyrophosphate. Tetrasilver thiopyrophosphate ($P_2S_7^{4\ominus}$), 8CI
[39473-22-8]

$Ag_4P_2S_7$

M 717.8
Synth. from Ag + P + S in quartz ampoule at 350-600°. Monoclinic yellow cryst. Dec. at *ca.* 470°.

Toffoli, P. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1492 (*synth, cryst struct*)
Voroshilov, Yu.V. *et al*, *CA*, 1977, **86**, 36595.
Andrae, H. *et al*, *J. Therm. Anal.*, 1989, **35**, 595 (*synth, phase diagram, props*)

Ag_5IO_6 IC-000090
Silver periodate (Ag_5IO_6)
[15122-61-9]

Ag_5IO_6

M 762.2
Precipitated from solns. of $Ag^{\oplus}$ + periodate. Commercially available. Black cryst. Insol. H_2O.

Gyani, P.P., *J. Indian Chem. Soc.*, 1950, **27**, 5 (*synth*)
Souchay, P. *et al*, *Bull. Soc. Chim. Fr.*, 1953, 599 (*synth*)

$Ag_6O_7Si_2$ IC-000091
Silver silicate ($Ag_6(Si_2O_7)$)
Silver pyrosilicate
[65161-09-3]

$Ag_6[Si_2O_7]$

M 815.3
Cryst. Angle: SiOSi 137.9°.

Jansen, M., *Acta Crystallogr., Sect. B*, 1977, **33**, 3584 (*cryst struct*)
Friebel, C. *et al*, *Z. Naturforsch., B*, 1984, **39**, 739.

Ag_8GeS_6 IC-000092
Silver germanide sulfide (Ag_8GeS_6)
Germanium silver sulfide ($GeAg_8S_6$), 9CI
[12250-22-5]

Ag_8GeS_6

M 1127.9
Compd. in which the element germanium was discovered. Prepd. by addition of $Ag^{\oplus}$ to a soln. of GeS_2 in Na_2S. Cryst. Exists in a high-temp. cubic form (argyrodite) and a low-temp. orthorhombic form (synthetic argyrodite). Semiconductor. Mp 955°.
Mineral-form [12250-23-6]
Argyrodite
Found in Bolivia, Germany and Utah. Steel-grey with reddish tint, orthorhombic cryst. Rapidly tarnishes black with purple or bluish tint.

Schwarz, R. *et al*, *Ber., B*, 1929, **63**, 778 (*synth*)
Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1944, **1**, 356 (*mineral*)
Hahn, H. *et al*, *Naturwissenschaften*, 1965, **52**, 451 (*cryst struct*)
Gorochov, O., *Bull. Soc. Chim. Fr.*, 1968, 2263 (*polymorphs*)
Eulenberger, G., *Monatsh. Chem.*, 1977, **108**, 901 (*cryst struct, orthorhombic*)

Ag_8GeSe_6 IC-000093
Silver germanide selenide (Ag_8GeSe_6)
[12250-24-7]

Ag_8GeSe_6

M 1409.3
Rhombohedral pseudocubic single crystals. Anion lattice consists of 3-D connected polyhedra with coordination nos. 12 and 16. Isolated $GeSe_4$ tetrahedra have $Ag^{\oplus}$ distributed over a no. of sites with distorted tetrahedral, trigonal or linear coordination. Steel grey cryst.

Bendonus, R. *et al*, *Phys. Status Solidi A*, 1975, **28**, K125 (*ir*)
Uutemichter, J. *et al*, *Z. Naturforsch., B*, 1978, **33**, 866 (*cryst struct*)
Ollitrault-Fichet, R. *et al*, *J. Less-Common Met.*, 1985, **114**, 273.

Ag_8S_6Sn IC-000094
Silver tin sulfide (Ag_8SnS_6)
[12250-27-0]

Ag_8SnS_6

M 1174.0
Cryst. Mp 839°.
Mineral-form
Canfieldite
May also be formulated as $Ag_8(Sn,Ge)S_6$. Occurs as mineral at sites in S. America, Europe and Japan, associated with other silver minerals. Steel grey cubic cryst. with reddish tinge; rapidly tarnishes becoming black with purple or bluish tint.

Hahn, H. *et al*, *Naturwissenschaften*, 1965, **52**, 451.
Gorochov, O., *Bull. Soc. Chim. Fr.*, 1968, 2263 (*cryst struct, dta, synth*)
Katada, M., *J. Sci. Hiroshima Univ. Ser. A: Phys. Chem.*, 1975, **39**, 45 (*mössbauer*)
Van Unterrichter, J. *et al*, *Z. Naturforsch., B*, 1978, **33**, 866 (*cryst struct*)

$Ag_{10}O_{13}Si_4$ IC-000095
Silver silicate ($Ag_{10}(Si_4O_{13})$)
Silver oxide silicate ($Ag_{10}O(Si_4O_{12})$)
[70197-03-4]

$Ag_{10}[Si_4O_{13}]$

M 1399.0
Synthetic oligosilicate with unbranched four-fold tetrahedra. Vermilion powder or triclinic cryst.

Jansen, M. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1979, **18**, 464 (*cryst struct*)

Al IC-000096
Aluminium
Aluminum, 9CI
[7429-90-5]

Al

M 26.9
Atomic No. 13. Ground state electron config. $[Ne]3s^23p^1$. 8 Isotopes reported of which only ^{27}Al is natural and stable. Discovered in 1825 by H.C. Oersted (Copenhagen) and first obt. electrolytically by C.M. Hall (1886). Abundance: 83,000 ppm (earth's crust), 0.01 ppm (sea water). Has fcc struct. Most abundant metallic element on surfaces of earth and moon. Common constit. of many igneous minerals incl. kaolin, bauxite, feldspars, micas, and occurs in many gemstones (ruby, sapphire, emerald). Metal obt. commercially from bauxite by purifn., dehydration and electrolysis of soln. in molten cryolite. (Hall-Héroult process) or by electrolysis of molten $AlCl_3$ (Alcoa process). Widely used in transport, construction. In electrical cables, busbars. In storage tanks, reflectors for radiant heat. As finisher in steel industry. Finely divided in thermite, paints, explosives. Implicated in Alzheimer's disease. Hard, strong, silvery-white metal: in bulk form protected from oxidation in air by coherent Al_2O_3 coating. Sol. alkalis; when finely divided, sol. hot H_2O. Mp 660.4°. Bp 2494° (2467°). Reduces many oxides to the free metal (cf. thermite welding process). Reacts with S, P, N at high temps: with C at 1000°. V. pure Al is resistant to most acids (except aqua regia). Halogens react vigorously with Al. Superconductor near abs. zero.
▷ BD0330000.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1923, **5**, 148 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 35, 1934-1950 (*rev, bibl*)
Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th ed., 1956, 565 (*history*)
Willardson, R.K. *et al*, *Compound Semiconductors*, Reinhold, 1962, 59 (*synth*)
Altenpohl, D., *Aluminium und Aluminiumlegierungen*, Springer, Berlin, 1965.
van Lancker, M., *Metallurgy of Aluminium Alloys*, Chapman and Hall, London, 1967.
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 993 (*rev*)
McGuire, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Nicholls, C.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 901 (*x-ray emission*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 129 (*rev, bibl*)
Polmear, I.J., *Light Alloys*, Edward Arnold, London, 1980
Russell, A.S., *Metall. Trans. B*, 1981, **12**, 203 (*manuf*)
Kidd, R.G., *NATO ASI Ser., Ser. C*, 1983, **103**, 329 (*Al-27 nmr*)
Delpuech, J.J., *NMR Newly Accessible Nuclei*, (Ed. Laszlo, P.), Academic Press, N.Y., 1983, **2**, 153 (*Al-27 nmr*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 243 (*rev*)
Jarrett, N., *Metall. Trans. B*, 1987, **18**, 289 (*manuf*)

Prod. Alum. and Alumina, 1987, (A.R. Burkin, Ed.), Wiley, 1987.
Hercock, R.L., *J. Am. Chem. Soc.*, 1989, **111**, 8582 (*rec*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 14.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 134 (*haz*)
Brethcick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 20 (*haz*)

IC-000097

AlAs

Aluminium arsenide (AlAs)

[22831-42-1]

AlAs

M 101.9
Zinc blende struct. From As_2/H_2 and Al at 1100° or from elements at 600°. Orange moisture sensitive cryst. (molten Al). Insol. Me_2CO, C_6H_6. Mp 1740°. ΔH_f° –146.5 kJ mol^{-1}, E_g^* 2.25 eV.

Semiconducting III-V Compounds, Hilsum, C., *et al*, Pergamon, Oxford, 1961.
Compound Semiconductors, Willardson, R.K., *et al*, Reinhold, 1962 (*synth*)
Kischio, W., *Z. Anorg. Allg. Chem.*, 1964, **328**, 187 (*synth, props*)
O'Keefe, M. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3519 (*cryst struct*)

IC-000098

$AlAsO_4$

Aluminium arsenate ($AlAsO_4$)

[13462-91-4]

$AlAsO_4$

M 165.9
Precipitated from K_2HAsO_4 + $Al_2(SO_4)_3$. Several hydrates descr.

Compd. with ethanolamine (2:1):
$C_4H_{14}Al_2As_2NO_8$ M 392.8
Synth. from ethanolamine, Al_2O_3, As_2O_5 and H_2O at 200° for 4 d. White cryst. (H_2O). Struct. with 3-D open framework with channels of 8 octahedrally coord. Al and tetrahedrally coord. As in one direction.

Hexagonal-form
Quartz struct. Obt. by heating pptd. compd. to 250°.

Tetragonal-form
High-pressure-form
Rutile struct. Formed from Al_2O_3, As_2O_5 at 8.9×10^4 atm., 900°. An orthorhombic form has also been descr.

Sharan, B., *Acta Crystallogr.*, 1959, **12**, 948 (*powder struct*)
Martin, R. *et al*, *Bull. Soc. Chim. Fr.*, 1959, 412 (*hydrates*)
Young, A.P. *et al*, *Z. Kristallogr.*, 1963, **118**, 223 (*high press form*)
Guanghi Yang, *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 810 (*synth, cryst struct, $AlAsO_4$*)

[AlB] IC-000099

Aluminium borides

[37367-77-4]

At least four phases known. AlB_2, AlB_{12} are commercially available.

Aluminium boride* (AlB_2), *9CI, 8CI [12041-50-8]
Aluminium diboride
AlB_2 M 48.6
Struct. has hexagonal nets of B atoms each surrounded by 6 Al at corners of trigonal prisms. Synth. from H_3BO_3, (or KBF_4) + Al at 800-1300° or Al + B_2O_3/KCl at 1200°. Black cryst. platelets with metallic lustre, or needles (hexagonal stars). Mp *ca.* 1350°. Metallic conductor: 333 Ω^{-1} m^{-1}. When finely divided, begins to oxidise in air at 700-800°. Dec. at *ca.* 1350° → AlB_{12} + B. Reacts slowly with H_2O, aq. HCl.

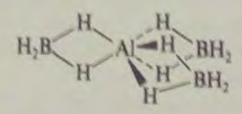
***Aluminium boride* (AlB_4)** [111050-36-3]
AlB_4 M 70.2
Struct. has chains of B_6 octahedra joined by B_2 with Al in tunnel-like cavities. Dark solid, not well-characterised.

Aluminium boride* (AlB_{12}), *9CI, 8CI [12041-54-2]
Aluminium dodecaboride
AlB_{12} M 156.7
Exists in α (tetragonal) and γ (orthorhombic) modifications. 'β-Phase' contains C. α-Form contains 3-D array of B_{12} icosahedra, B_{10} units and single B atoms. The B_{10} units are twinned icosahedra with triangular plane and vacant apex on each side. B sites in ratio 2:1:1. Al atoms distributed statistically. Synth. from Al + $Na_4B_4O_7$ at 1000-1100°; or Al + B at 1100-1200°. Employed in manuf. of lightweight armour plate; also catalyst for org. reactions. Yellow to brown acicular prisms or tetragonal bipyramids. Mp *ca.* 2070°. When finely divided, begins to oxidise in air at *ca.* 650°. Dec. to AlB_2 at 1350-1450°. α-form stable 1000-2000°. Band gap E_g^* 1.8-1.9 eV.

[12280-42-9]
Felten, E.J., *J. Am. Chem. Soc.*, 1956, **78**, 5977 (*cryst struct, AlB_2*)
Duhart, P., *Ann. Chim. (Paris)*, 1962, **7**, 339 (*rev, synth, props*)
Matkovich, V.I. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 2337 (*synth, props*)
Greenwood, N.N. *et al*, *Q. Rev., Chem. Soc.*, 1966, **20**, 441 (*rev*)
Serebryanskii, V.T. *et al*, *Zh. Neorg. Khim.*, 1967, **12**, 2486; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 1311 (*synth, phase diagram*)
Economy, J., *Chem. Eng. Progress*, 1969, **65**, 46 (*use, rev*)
Neronov, V.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 896 (*phase diagram*)
Kopp, J.P. *et al*, *J. Chem. Phys.*, 1971, **54**, 1840 (*B-11 nmr, Al-27 nmr*)
Sirtl, E. *et al*, *J. Crystal Growth*, 1972, **16**, 215 (*synth, props*)
Mavel, G. *et al*, *Surf. Sci.*, 1973, **35**, 109 (*pe*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 788 (*synth*)
Hughes, R.E. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 5507 (*cryst struct*)
Higashi, I. *et al*, *J. Solid State Chem.*, 1977, **20**, 67 (*synth, cryst struct*)
Kasper, J.S. *et al*, *J. Solid State Chem.*, 1977, **20**, 281 (*synth, cryst struct*)
McKee, D.W., *Carbon*, 1986, **24**, 331 (*props*)

AlB_3H_{12} IC-000100

Aluminium(*III*) borohydride
Tris[tetrahydroborato(1–)-H,H']aluminium
[13771-22-7]



M 71.5
Molecular struct. (D_{3h}) maintained in solid, liquid and gas phases. Synth. from $NaBH_4$ and $AlCl_3$. Colourless pyrophoric moisture sensitive liq. d 0.55. V.p. 119.5 mm/0°. Dec. slowly giving H_2.

▷ May detonate in moist air.

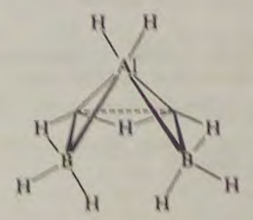
Schlesinger, H.I. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 209 (*synth, props*)
Almenningen, A. *et al*, *Acta Chem. Scand.*, 1968, **22**, 328 (*ed*)

Lauterbur, P.C. *et al*, *Inorg. Chem.*, 1968, **7**, 1025 (*B-11 nmr, Al-27 nmr*)
Coe, D.A. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 1789 (*ir, raman, pmr*)
Titov, L.V. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1974, **23**, 2410 (*Al-27 nmr*)
Boiko, G.N. *et al*, *Usp. Khim.*, 1975, **44**, 3 (*pmr, B-11 nmr, rev*)
Semenenko, K.N. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1978, **27**, 994 (*complexes*)

AlB_4H_{11} IC-000101

Dihydro[η^4-nonahydrotetraborato(1–)]aluminium, 10Cl

[76797-41-6]



M 81.3
Obt. from Aluminium(*III*) borohydride, IC-000100 and B_2H_6. Amorph. white solid. Dec. >140°. Insol. C_6H_6, hexane.

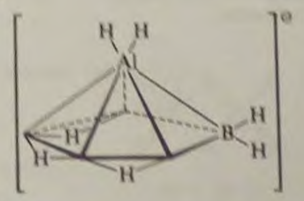
▷ Pyrophoric.

Himpsl, F.L. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 1098 (*synth, ir, powder struct*)

$AlB_5H_{11}^{\ominus}$ IC-000102

Dihydro[η^4-nonahydropentaborato(2–)]aluminate(1–), 10Cl

[76797-37-0]



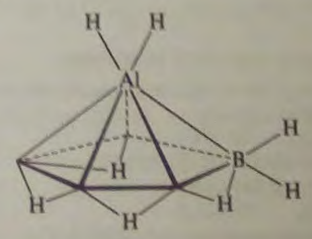
M 92.1 (ion)
Proposed struct. shown. By reaction of AlB_4H_{11} with $BH_4^{\ominus}$ in diglyme. No phys. props. reported.

Himpsl, F.L. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 1098 (*synth*)

AlB_5H_{12} IC-000103

[η^4-Decahydropentaborato(1–)]dihydroaluminium

[76797-40-5]



M 93.1
From Aluminium(*III*) borohydride, IC-000100 and B_5H_9. Light yellow air- and moisture-sensitive amorph. solid. Insol. C_6H_6.

Himpsl, F.L. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 1098 (*synth, ir*)

$AlB_6H_{12}^{\ominus}$ IC-000104

Dihydro[η^4-decahydrohexaborato(2–)]aluminate(1–), 10Cl

[76797-36-9]

$[AlB_6H_{12}]^{\ominus}$

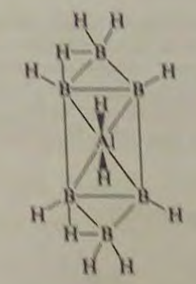
M 103.9 (ion)
arachno class, struct. unknown. Synth. by reaction of AlB_5H_{12} with $BH_4^{\ominus}$ in diglyme. Not isol.

Bond, A.C. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 1098 (*synth*)

AlB_6H_{13} IC-000105

Dihydro[η^4-undecahydrohexaborato(1–)]aluminium, 10Cl

[76797-39-2]



proposed struct.

M 104.9
Obt. by dec. of $(BH_4)Al(B_3H_8)_2$ at 100°. Possesses exceptionally high thermal stability. White solid.

▷ Pyrophoric.

Bond, A.C. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 1098 (*synth, ir*)

$AlB_8O_{15}^{3\ominus}$ IC-000106

Aluminononaborate(3–), 11Cl

$[AlB_8O_{15}]^{3\ominus}$

M 353.4 (ion)
Contains B_3O_3 – triborate and B_5O_6 – pentaborate groups bonded via AlO_4 tetrahedra in an infinite 2D double layer struct.

Tri-K salt: [84067-38-9].
Colourless cryst.

Tanaka, Y. *et al*, *CA*, 1983, **98**, 21013 (*synth, cryst struct*)

[AlBa] IC-000107

Aluminium-barium system

***Aluminium barium* (Al_2Ba_3)** [117248-52-9]
Al_2Ba_3 M 546.8
From metals at 1000°. Metallic cryst. (melt).

Fornasini, M.L. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 1355.

IC-000108

$AlBa_2F_8Zn$

Barium μ-fluorotetrafluoro(tetrafluoroaluminate)zincate(4−)

Aluminium barium zinc fluoride ($AlBa_2ZnF_8$)

[34667-67-4]

$Ba_2[AlZnF_8]$

M 538.0

MF_6 octahedra with statistical distributions of Zn, Al at M sites are linked through corners to stair-like framework. Synth. from BaF_2, ZnF_2 and AlF_3 in F_2 at 550-750°. Colourless moisture sensitive cryst. (melt).

Fleischer, T. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **492**, 83 (*synth, cryst struct*)

IC-000109

$AlBe_2Ca_2KO_{30}Si_{12}$

Milarite

[12251-59-1]

$KCa_2AlBe_2(Si_{12}O_{30}).H_2O$

M 981.2

Unbranched, dicyclosilicate (6 SiO_4 tetrahedra per ring). Also formulated as $KCa_2(Be,Al)_3[Si_{12}O_{30}].0.75H_2O$. Mineral. Pale green transparent cryst.

Povarennykh, A.S., *Mineral. Zh.*, 1979, **1**, 3 (*ir*)
Černý, P. *et al*, *Can. Mineral.*, 1980, **18**, 41 (*cryst struct*)
Janeczek, J., *Mineral. Mag.*, 1986, **50**, 271 (*cryst struct*)

IC-000110

AlBr

Aluminium(*I*) bromide (AlBr)

[22359-97-3]

AlBr

M 106.8

Unstable sp. studied in gas phase or in Ne or Ar matrices. From Al(g)/Ar + Br_2 or generated in graphite furnace. Species for detn. of traces of Br. ΔH°_{f298} AlBr(g) +15.1 kJ mol^{-1}; S° 239.5 J K^{-1} mol^{-1}.

Rosenwaks, S., *J. Chem. Phys.*, 1976, **65**, 3668 (*ir*)
Schnöckel, H., *Z. Naturforsch., B*, 1976, **31**, 1291 (*synth, ir*)
Tsunoda, K. *et al*, *Anal. Chem.*, 1978, **50**, 861 (*use*)
Tsunoda, K. *et al*, *Spectrochim. Acta, Part B*, 1980, **35**, 715 (*ir*)

AlBrO IC-000111

Aluminium(*III*) bromide oxide (AlBrO)

[13596-10-6]

AlOBr

M 122.8

Struct. with alternate Al—O and Br layers. From As_2O_3 + $AlBr_3$ in sealed tube. White moisture sensitive cryst. Dec. >460°.

Hagenmuller, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1961, **252**, 282 (*synth, props*)
Hagenmuller, P. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **323**, 1 (*synth, powder struct*)
Batsanov, S.S. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1968, **9**, 282 (*rev*)

AlBrS IC-000112

Aluminium bromide sulfide (AlBrS)

Aluminium(III) *sulfide bromide*

AlSBr

M 138.9

Synth. from Al_2S_3 + $AlBr_3$ in sealed tube. White v. hygroscopic needles. Insol. org. solvs.

Hagenmuller, P. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **323**, 1 (*synth, powder struct*)
Lin Zhengyan, *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 67 (*synth, ir, raman*)

IC-000113

AlBrSe

Aluminium(*III*) bromide selenide (AlBrSe)

[29758-55-2]

AlBrSe

M 185.8

Synth. from Al_2Se_3 + $AlBr_3$. V. hygroscopic white powder. Insol. Et_2O, C_6H_6, THF, CS_2, CCl_4.

Palvadeau, P. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 2698 (*synth, powder struct, props*)
Lin Zhengyan, *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 67 (*synth, powder struct, raman, ir*)

IC-000114

AlBrTe

Aluminium(*III*) bromide telluride (AlBrTe)

AlBrTe

M 234.4

Synth. from $AlBr_3$ + Al_2Te_3 or $AlBr_3$ + ZnTe in sealed tube at 350°. Poorly cryst. creamy v. hygroscopic powder. Insol. Et_2O, EtOH, Me_2CO, C_6H_6, $CHCl_3$, CCl_4.

Rouxel, J. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2044 (*synth, props*)

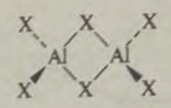
IC-000115

$AlBr_3$

Aluminium(*III*) bromide ($AlBr_3$)

Aluminium tribromide

[7727-15-3]



Dimer

X = Br

M 266.6

Dimeric molecular structure in solid, liq. and oligomeric $(AlBr_3)_n$ n = 1,2,4,6 in gas. Monomer studied in Ar matrix. Synth. from elements at 100°. Lewis acid. Friedel Crafts catalyst. Catalyst for alkane isom. Agent for chemical transport in metal halide synth. Commercially available. Forms many complexes with Lewis bases and weak adducts with aromatic hydrocarbons, alkenes and alkynes. ΔH_f°(s) −494.8 kJ mol^{-1} (per $AlBr_3$). $\Delta H_{f\ 298}^\circ$ −527.2 kJ mol^{-1}; S° 180.2 J K^{-1} mol^{-1}.

▷ Reacts violently with H_2O. BD0350000.

Hexahydrate: [7784-11-4]. *Hexaaquaaluminium(3+) tribromide*
$AlBr_3H_{12}O_6$ M 374.7
Colourless needles (H_2O). Mp 93°.

C_6H_6 complex: [6736-24-9].
$C_6H_6Al_2Br_6$ M 611.5
Colourless air sensitive cryst. (C_6H_6). C_6H_6 and Al_2Br_6 present in cryst. Similar compds. with toluene and xylenes descr.

$SbBr_3$ complex: see *Tribromo(tribromostibine)aluminium*, *IC-000119*

Dimer: Di-μ-bromotetrabromodialuminium
Al_2Br_6 M 533.3
Colourless moisture-sensitive hexagonal plates. In presence of HBr reacts slowly with aliphatic hydrocarbons. Sol. C_6H_6, CS_2, hexane. Mp 97°. Bp 250-270°.

Kendall, J. *et al*, *J. Am. Chem. Soc.*, 1923, **45**, 963 (*phase diagram*)
Renes, P.A., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1945, **64**, 275 (*cryst struct*)
Inorg. Synth., 1950, **3**, 30 (*synth*)
Walker, D.G., *J. Phys. Chem.*, 1960, **64**, 939 (*complexes*)
Eley, D.D. *et al*, *J. Chem. Soc.*, 1961, 3867 (*cryst struct, C_6H_6 complex*)
Walter-Lévy, L. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1963, **256**, 1786 (*tga*)
Greenwood, N.N. *et al*, *Friedel-Crafts Rel. Reacts.*, (Ed. Olah, G.A.), Wiley, N.Y., 1963.
Sang Up Choi, *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 903, 4128 (*arene complexes*)
Wilson, J.W. *et al*, *J. Chem. Soc. A*, 1967, 392; 1968, 316, 2389 (*complexes*)
Bliznakov, G. *et al*, *J. Less-Common Met.*, 1967, **12**, 405 (*synth*)
Beattie, I.R., *J. Chem. Soc. A*, 1968, 813; 1969, 2655 (*ir, raman*)
Haraguchi, H. *et al*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
O'Brien, J.F., *J. Phys. Chem.*, 1970, **74**, 743 (*complexes*)
Okuda, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2245 (*nqr*)
McGuire, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Anthoney, M.E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 659 (*thermodyn*)
Lappert, M.F. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1976, **72**, 539 (*pe*)
Olah, G.A. *et al*, *J. Org. Chem.*, 1977, **42**, 4187 (*use*)
Schäfer, H. *et al*, *J. Less-Common Met.*, 1978, **61**, 47 (*use*)
Pong, R.G.S. *et al*, *J. Chem. Phys.*, 1979, **70**, 525 (*ir*)
Dalibart, M. *et al*, *Inorg. Chem.*, 1981, **20**, 3975 (*complexes*)
Imamura, H. *et al*, *Z. Phys. Chem. Neue Folge*, 1981, **125**, 251.
Martin, T.P. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 623 (*ms*)
Dalibart, M. *et al*, *Coord. Chem. Rev.*, 1986, **74**, 1 (*complexes*)
Sanders, J.R. *et al*, *J. Electrochem. Soc.*, 1986, **133**, 325 (*complexes, use*)

$AlBr_3O_9$ IC-000116

Aluminium bromate ($Al(BrO_3)_3$)

$Al(BrO_3)_3$

M 410.6

Obt. as nonahydrate.

Nonahydrate:
$AlBr_3H_{18}O_{18}$ M 572.8
From $Al(SO_4)_3$ and $Ba(BrO_3)_2$. Sl. hygroscopic white cryst. (H_2O). Mp 62°.

Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 1058.

$AlBr_4^\ominus$ IC-000117

Tetrabromoaluminate(1−)

[22602-42-2]

$[AlBr_4]^\ominus$

M 346.5 (ion)

Species $[AlCl_nBr_{4-n}]^\ominus$ also descr.

Li salt: [15003-50-6]. *Lithium tetrabromoaluminate* (*$LiAlBr_4$*)
$AlBr_4Li$ M 353.5
From LiBr + $AlBr_3$ in EtBr. White moisture-sensitive cryst. Mp 195°.

Na salt: [23630-67-3]. *Sodium tetrabromoaluminate* (*$NaAlBr_4$*)
$AlBr_4Na$ M 369.5
From NaBr + $AlBr_3$ in EtBr. White moisture-sensitive cryst. Mp 199°.

K salt: [18041-28-6]. *Potassium tetrabromoaluminate* (*$KAlBr_4$*)
$AlBr_4K$ M 385.6
From KBr + $AlBr_3$ in C_2H_5Br. White moisture-sensitive cryst. Mp 192°. Two modifications descr.

Rb salt: [18041-29-7].
$AlBr_4Rb$ M 432.0
Obt. from RbBr-$AlBr_3$ melt. White moisture-sensitive cryst. Mp 278°.

Cs salt: [18041-30-0].
$AlBr_4Cs$ M 479.5
Obt. from CsBr-$AlBr_3$ melt. White moisture-sensitive cryst. Mp 357°.

Me_4N salt: [22578-15-0].
From $[Me_4N]Br$ + $AlBr_3$ in CH_2Br_2. Colourless moisture sensitive cryst. (CH_2Br_2/cyclohexane). Et_4N salt also descr.

Cronenberg, C.T.H.M. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **354**, 103 (*synth, phase diagram*)
Mikheeva, V.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 884 (*phase diagram*)
Kinsella, E. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 2139 (*ir*)
Haraguchi, H. *et al*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
Brown, D.H. *et al*, *Spectrochim. Acta, Part A*, 1970, **26**, 1344.
Begun, G.M. *et al*, *Inorg. Chem.*, 1971, **10**, 886 (*raman*)
Vandorpe, B. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **275**, 487 (*synth, props*)
Okuda, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 3136 (*nqr*)
Tarasov, V.P. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1978, **19**, 866 (*Al-27 nmr*)
Dubois, B. *et al*, *C.R. Hebd. Seances Acad. Sci., Ser. 2*, 1981, **292**, 517 (*Me_4N salt*)
Dalibart, M. *et al*, *Inorg. Chem.*, 1981, **20**, 3975 (*ir, raman, Al-27 nmr*)
Wehrli, F.W. *et al*, *J. Magn. Reson.*, 1981, **44**, 197 (*Al-27 nmr*)

$AlBr_4In$ IC-000118

Indium(1+) tetrabromoaluminate(1−)

[67297-49-8]

$In[AlBr_4]$

M 461.4

May be important in chemical vapour transport. White moisture sensitive solid. Mp 200°.

Radloff, P.L. *et al*, *J. Chem. Phys.*, 1980, **72**, 992 (*synth, raman*)

$AlBr_6Sb$ IC-000119

Tribromo(tribromostibine)aluminium

Aluminium(III) *bromide antimony*(III) *bromide*

[24508-60-9]

$Br_3AlSbBr_3$

M 628.1

White moisture sensitive cryst. (melt). Mp 85°.

Spiridonov, V.P. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1969, **10**, 303 (*ed*)
Okuda, T. *et al*, *Chem. Lett.*, 1975, 785 (*nqr*)
Kendall, J. *et al*, *J. Am. Chem. Soc.*, 1923, **45**, 963 (*phase diagram*)

$AlCaNaO_7Si_2$ IC-000120

Melilite

[12003-56-4]

$CaNaAl[Si_2O_7]$

M 258.2

Mineral. Cryst.

[12173-94-3]

Sabana, Th.G. *et al*, *Bull. Comm. Geol. Finl.*, 1967, **229**, 29 (*ir*)
Louisnathan, S.J., *Z. Kristallogr.*, 1970, **131**, 314 (*synth, cryst struct*)

IC-000121

$AlCa_2H_8O_{12}Si_4$

Gismondine
Gismondite (improper)
[12251-23-9]

$Ca_4[Al_8Si_8O_{32}].16H_2O$

M 363.3
Zeolite struct. GIS with chains of $(Al,Si{-}O)_4$ or $(Al,Si{-}O)_8$ rings giving 3D system of elliptical channels (310 × 450 or 280 × 490 pm across). Member of phillipsite group. Mineral found in Israel, Senegal, Australia, USA, Ireland, Rome, Iceland, Czechoslovakia and Faeroe Islands. White cryst. Related minerals Amicite and Gobbinsite also descr.

Me_4N-form:
$C_8H_{16}AlNO_8Si_3$ M 331.3
Synthetic zeolite obtained hydrothermally at 130°. White cryst. Absorbs var. amts. H_2O. Formulated as e.g. $Me_4NAlSi_3O_8.H_2O$.

Mineral-form:
$Al_2CaH_8O_{12}Si_4$ M 350.2
Rather rare zeolite of hydrothermal origin; occurs in cavities of massive rocks. Colourless to white or grey solid.

[1318-56-5]

Fischer, K., *Am. Mineral.*, 1963, **48**, 664 (*cryst struct*)
Baerlocher, C. *et al*, *Helv. Chim. Acta*, 1970, **53**, 1285; *Z. Kristallogr.*, 1972, **135**, 339 (*synth, cryst struct*)
Alberti, A. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2866 (*cryst struct, amicite*)
Wirsching, U., *Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Barrer, R.M., *Hydrothermal Chemistry of Zeolites*, Academic Press, London, 1982.
Gottardi, G. *et al*, *Natural Zeolites*, Springer, 1985, 122 (*synth, props*)
McCusker, L.B. *et al*, *Z. Kristallogr.*, 1985, **171**, 281 (*cryst struct, gobbinsite*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 1730 (*Al-27 nmr*)
Artioli, G. *et al*, *Zeolites*, 1986, **6**, 361 (*nd*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 66.

$AlCa_7H_{10}NaO_{36}Si_{11}$ IC-000122

Reyerite, 9Cl
[12424-04-3]

$(Na,K)Ca_7[Si_4O_{10}][(AlSi_7)O_{19}](OH)_4.3H_2O$

M 1225.5
Mineral. An unbranched double layer silicate. Also formulated as $(Na,K)_4Ca_{14}(Si,Al)_{24}O_{60}(OH)_5.5H_2O$. First collected at Niakornak, Greenland. Colourless thin plates.

Chalmers, R.A. *et al*, *Mineral. Mag.*, 1964, **33**, 265 (*mineral*)
Clement, S.C. *et al*, *Am. Mineral.*, 1973, **58**, 517 (*occur, props*)
Merlino, S., *Mineral. Mag.*, 1988, **52**, 247 (*cryst struct*)

AlCl IC-000123

Aluminium(*I*) chloride (AlCl)
[13595-81-8]

AlCl

M 62.4
Studied spectroscopically in gas phase or noble gas matrices; Al—Cl 212.9 pm. From Al + $AlCl_3$ (427-727°) or Al + HCl (927°). Gas-phase species used for determination of traces of Cl. Dark red, extremely air- and moisture-sensitive solid at −196°. Dec. → Al + $AlCl_3$ > −93°. Sol. Et_2O, toluene. Ir ν_{Al-Cl} 477 cm^{-1} (gas); 450 cm^{-1} (Et_2O/toluene < −113°). ΔH_f° AlCl(g) −51.5 kJ mol^{-1}; S° 227.8 J K^{-1} mol^{-1}.

Foster, L.M. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 2580 (*synth, uv, thermodyn data*)
Russell, A.S. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 1466 (*thermodyn data*)
Lide, D.R., *J. Chem. Phys.*, 1965, **42**, 1013 (*microwave*)
Rosenwaks, S., *J. Chem. Phys.*, 1976, **65**, 3668 (*uv*)
Schnöckel, H. *et al*, *Z. Naturforsch., B*, 1976, **31**, 1291 (*synth, ir*)
Tsunoda, K. *et al*, *Anal. Chem.*, 1978, **50**, 861 (*use*)
Tsunoda, K. *et al*, *Spectrochim. Acta, Part B*, 1980, **35**, 715 (*uv*)
Tacke, M. *et al*, *Inorg. Chem.*, 1989, **28**, 2895 (*ir, Al-27 nmr*)

$AlClCuH_{28}O_{12}S_2$ IC-000124

Aubertite
Aluminium copper(II) chloride sulfate tetradecahydrate
[71768-27-9]

$[Al(OH_2)_6][Cu(OH_2)_6][SO_4]_2Cl.2H_2O$

M 570.3
Lattice of discrete ions held by H-bonds. Mineral (Chile). Bluish green solid. $Cu_6Al(SO_4)(OH)_{12}Cl.3H_2O$. Spangolite also descr.

Ginderow, D. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2499 (*cryst struct*)

$AlClH_2$ IC-000125

Aluminium chloride hydride ($AlClH_2$)
Chloroalane
[14644-71-4]

$AlClH_2$

M 64.4
From $LiAlH_4$ and $AlCl_3$ (1:1). Reducing agent for alkenes and ketones. Usually used *in situ*.

Me_3N complex: [6401-80-5]. *Chlorodihydro(trimethylamine) aluminium. Chloro(N,N-dimethylmethanamine) dihydroaluminium*
$C_3H_{11}AlCl$ M 109.5
From Me_3NAlH_3 + $HgCl_2$. White v. moisture-sensitive solid (by subl.). Mp 51-52°. $Bp_{0.01}$ 40°.

Et_3N complex: [12106-60-4]. *Chlorodihydro(triethylamine) aluminium. Chloro(N,N-diethylethanamine) dihydroaluminium*
$C_6H_{17}AlCl$ M 151.6
From $LiAlH_4$ + $AlCl_3$ + Et_3N. Colourless air- and moisture-sensitive liq. Sol. C_6H_6. Mp −6° to −4°.

Ruff, J.K. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 1798 (*synth*)
Ashby, E.C. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 729 (*synth*)
Inorg. Synth., 1967, **9**, 30 (*synth*)
Yoshio, M. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 2439; **36**, 2314 (*conductivity*)
Semenenko, K.N. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 1921 (*props*)
Ashby, E.C. *et al*, *J. Org. Chem.*, 1979, **44**, 4364 (*use*)

AlClO IC-000126

Aluminium chloride oxide (AlClO)
Aluminium(III) oxide chloride
[13596-11-7]

AlClO

M 78.4
Struct. comprises alternate Al—O and Cl layers Al 6- O 4- Cl 2-coord. Synth. from $AlCl_3$ and Sb_2O_3. Moisture sensitive white solid. $\Delta H_{f,\,298}^\circ$ −795 kJ mol^{-1}; S° 54.3 J K^{-1} mol^{-1}. Also isolated in Ar matrices, AlFO similarly.

Schäfer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **297**, 48 (*synth, props*)
Rouxel, J. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **248**, 810 (*synth, props*)
Hagenmuller, P. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **323**, 1; 1967, **355**, 209 (*synth, powder struct, reactions*)
Batsanov, S.S. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1968, **9**, 282 (*rev*)
Srivastava, R.D. *et al*, *J. Phys. Chem.*, 1971, **75**, 1760 (*ms*)
Morozov, A.I. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 659 (*synth, props*)
Schnöckel, H. *et al*, *J. Mol. Struct.*, 1978, **50**, 267 (*matrix isol*)

AlClS IC-000127

Aluminium(*III*) chloride sulfide (AlClS)
[22847-28-5]

AlClS

M 94.5
Synth. from Al, S, $AlCl_3$ at 300°. Hygroscopic white needles.

Hagenmuller, P. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **323**, 1 (*synth, powder struct*)
Paulsen, K.A. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 6866 (*electrochemical data*)
Robinson, J. *et al*, *Inorg. Chem.*, 1977, **16**, 3040 (*electrochemical data*)
Berg, R.W. *et al*, *Inorg. Chem.*, 1980, **19**, 2688 (*synth, raman*)
Lin Zhengyan, *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 67 (*ir, raman*)

AlClSe IC-000128

Aluminium chloride selenide (AlClSe)
Aluminium(III) selenide chloride
[43337-67-3]

AlClSe

M 141.3
Synth. from $AlCl_3$, Al_2Se_3 at 350°. V. hygroscopic off white creamy powder. Insol. Et_2O, C_6H_6, THF, CS_2, CCl_4.

Palvadeau, P. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 2698 (*synth, powder struct*)
Robinson, J. *et al*, *Inorg. Chem.*, 1977, **16**, 3040 (*electrochem*)
Berg, R.W. *et al*, *Inorg. Chem.*, 1980, **19**, 2688 (*raman*)
Lin Zhengyan, *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 67 (*ir, raman*)

AlClTe IC-000129

Aluminium chloride telluride (AlClTe)
Aluminium(III) telluride chloride
[13824-68-5]

AlClTe

M 190.0
From $AlCl_3$ + Al_2Te_3 at 350° or from $AlCl_3$ + ZnTe at 400°. Creamy, v. moisture sensitive powder. Insol. Et_2O, EtOH, Me_2CO, C_6H_6, $CHCl_3$, CS_2, CCl_4.

Rouxel, J. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2044 (*synth, props*)
Robinson, J. *et al*, *Inorg. Chem.*, 1977, **16**, 3040 (*electrochem*)

$AlCl_2$ IC-000130

Aluminium(*II*) chloride ($AlCl_2$)
[16603-84-2]

$AlCl_2$

M 97.8
Isol. in Ar matrix or as unstable solid. From Al + $AlCl_3$ in heptane or *in vacuo* at 580°. May be intermed. in formation of alkylaluminium deriv.

Olah, G.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 3231 (*synth, ir*)

$AlCl_2H$ IC-000131

Aluminium chloride hydride ($AlCl_2H$)
Aluminium dichloride hydride. Dichloroalane
[13497-97-7]

$AlCl_2H$

M 98.8
From $LiAlH_4$ and $AlCl_3$ (1:3). Reagent for reduction of alkenes, ketones, cyclic ethers. Usually used *in situ*.

Et_3N complex: [17275-40-0]. *Dichlorohydro(triethylamine) aluminium, 8CI. Dichloro(N,N-diethylethanamine) hydroaluminium, 10CI*
$C_6H_{16}AlCl_2$ M 186.0
From $LiAlH_4$ + $AlCl_3$ + Et_3N. Colourless air and moisture sensitive solid (C_6H_6). Mp 45°.

Ashby, E.C. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 729 (*synth*)
Zajac, W.W. *et al*, *J. Org. Chem.*, 1970, **35**, 3375; 1972, **37**, 521 (*use*)
Loewen, P.C. *et al*, *Can. J. Chem.*, 1972, **50**, 1502 (*use*)
Yoshio, M. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 2439; 1976, **38**, 2314 (*conductivity*)
Ashby, E.C. *et al*, *Inorg. Chem.*, 1975, **14**, 1608 (*ir, use*)
Semenenko, K.N. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 1921 (*props*)
Schnöckel, H. *et al*, *J. Mol. Struct.*, 1978, **50**, 275 (*ir*)
Ashby, E.C. *et al*, *J. Org. Chem.*, 1979, **44**, 4364 (*use*)

$AlCl_3$ IC-000132

Aluminium(*III*) chloride ($AlCl_3$)
Aluminium trichloride
[7446-70-0]

$AlCl_3$

M 133.3
Distorted $CrCl_3$ struct. in solid state; dimeric in soln. and liq.; monomer, dimer and some trimer in vapour. Synth. from Al + Cl_2 or from Al + HCl at 500°. Lewis acid. Friedel Crafts catalyst. Intermed. in one process for manuf. of Al. Commercially available. Colourless hexagonal v. moisture sensitive plates. Mp 192° (2.5 atm). Subl. 180°. ΔH_f°(s) −705.8 kJ mol^{-1}; S° 109.2 J K^{-1} mol^{-1}. Many complexes descr.

▷ Reacts violently with H_2O. BD0525000.

Hydrate: [10124-27-3]. *Aluminium chloride hydrate*
Commercially available. A mixture of hydrated species $AlCl_3.x\,H_2O$.

Hexahydrate: [7784-13-6]. *Hexaaquaaluminium(3+) chloride*
$AlCl_3H_{12}O_6$ M 241.4
Salting agent in soap industry; component of deodorant prepns., wood preservative; in photofixing baths. Colourless cryst. (H_2O). Mp 100° dec.
▷ BD0530000.

NH_3 complex: see *Amminetrichloroaluminium, IC-000133*
Et_2O complex: [39624-48-1].

$(C_6H_{12}AlCl)_2$ M 207.6
White moisture sensitive plates (C_6H_6). Sol. C_6H_6, Et_2O; insol. cold hexane. Mp 30°. Mild (1) catalyst. Also dimer.

$(Bu_2AlCl_2NO)_2$ M 194.1
White moisture sensitive cryst. (C_6H_6/cyclohexane). Mp 87°.

$(Ph_2NO)_2$ complex:
$C_{24}H_{20}AlCl_2NO_2$ M 236.4
Bright yellow moisture sensitive cryst. ($CHCl_3$). Mp 75°.

Complex with nitrogen sulfide (N_2S_2) (1:1): [82557-52-0].
Bis(acetonitrile)(dimorpholinodithiolato-N,N')aluminium
$AlC_{12}N_4S_2$ M 156.8
Obt. from $AlCl_3$ and S_2N_2 in CH_2Cl_2. With S_2N_2 at 80° gives S_4N_4. Colourless air and moisture sensitive needles (CH_2Cl_2). Mp 151° dec.

Complex with nitrogen sulfide (N_2S_2): [38442-60-3].
$AlCl_3N_2S_2$ M 217.6
Obt. from S_2N_2 + $AlCl_3$ in 1,2-dichloroethane. Dark red air and moisture sensitive cryst. (1,2-dichloroethane).
Corresp. $AlBr_3$ adduct also descr.

Kazitsin, I.A.A., *Rec. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1947, **66**, 501 (*cryst struct*)
Harris, R.L. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 3151 (*x-ray liq*)
Klemperer, W., *J. Chem. Phys.*, 1956, **24**, 353 (*ir*)
Prasad-Cyril, *Rec. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1961, **80**, 1 (*ms*)
Jones, D.E.H. *et al*, *J. Chem. Soc. A*, 1966, 1448 (*complexes*)
Zaseeva, E.Z. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1967, **8**, 547 (*mol. structure*)
Mervin, W.G. *et al*, *J. Phys. Chem.*, 1968, **72**, 3063 (*solns in DMF*)
Boston, C.R., *J. Chem. Phys.*, 1969, **51**, 1669 (*elec cond*)
Harris, I.R. *et al*, *J. Chem. Soc. A*, 1969, 2655 (*ir, raman*)
Haraguchi, H. *et al*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
O'Brien, J.F. *et al*, *J. Phys. Chem.*, 1970, **74**, 743 (*solns in MeCN*)
Lesnicki, M.L. *et al*, *J. Chem. Phys.*, 1972, **56**, 4171; 1976, **64**, 910 (*ir, thermodyn props*)
McGuire, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Anthonsen, M.E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 659 (*thermodyn props*)
Nicholls, C.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 901 (*x-ray emission*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 826 (*synth, hexahydrate*)
Beattie, I.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 666; *J. Chem. Phys.*, 1976, **64**, 909 (*ir*)
Lappert, M.F. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1976, **72**, 539 (*pe*)
Schmidbaur, H., *Z. Anorg. Allg. Chem.*, 1976, **424**, 203 (*ir*)
Tranquille, M. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1980, **76**, 26 (*ir, raman*)
Bochkarev, V.N. *et al*, *Zh. Obshch. Khim.*, 1980, **50**, 586 (*ms*)
Thewalt, U. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 634 (*S,N complex*)
Nöth, H. *et al*, *Z. Naturforsch., B*, 1982, **37**, 29 (*Al-27 nmr*)
Hussey, C.L., *Adv. Molten Salt Chem.*, 1983, **5**, 185 (*complexes, use*)
Dahlhaus, M. *et al*, *Coord. Chem. Rev.*, 1986, **74**, 1 (*complexes*)
Benn, R. *et al*, *J. Organomet. Chem.*, 1987, **333**, 155 (*Al-27 nmr*)
Hoffmann, G.G., *J. Organomet. Chem.*, 1987, **335**, 143 (*complexes*)

$AlCl_3H_3N$ IC-000133

Aminetrichloroaluminium

Aluminium trichloride ammonia

[13550-09-3]

Cl_3AlNH_3

M 150.3
Monomeric in solid state. White moisture sensitive cryst. Mp 133°. Bp ~420°, Bp_1 195°. Forms solid solns. with $AlBr_3NH_3$.

Gerding, H. *et al*, *Rec. Trav. Chim. Pays-Bas U. R. Neth. Chem. Soc.*, 1953, **74**, 15 (*raman*)
Ramos, T., *Z. Anorg. Allg. Chem.*, 1959, **298**, 22 (*synth*)
Sawodny, W. *et al*, *Z. Phys. Chem. (Munich)*, 1965, **44**, 329 (*ir, raman*)
Grant, D.F. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 377 (*cryst struct*)
Mal'sin, L.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 1716 (*phase diagram*)
Ahmed, A. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **434**, 207 (*similar compds*)

$AlCl_3O_9$ IC-000134

Aluminium chlorate ($Al(ClO_3)_3$)

$Al(ClO_3)_3$

M 277.3
Hexahydrate. Colourless cryst. (H_2O).
▷ May react violently with filter paper.

Mishler, R.M., *Inorg. Chem.*, 1964, **3**, 199 (*nqr*)

$AlCl_3O_{12}$ IC-000135

Aluminium perchlorate ($Al(ClO_4)_3$)

[14452-39-2]

$Al(ClO_4)_3$

M 325.3
Synth. from $AlCl_3$ and $AgClO_4$ in C_6H_6. Commercially available. Aq. solns. source of Hexaaquaaluminium(3+), IC-000191. Similar species in DMF, dioxan, etc. White hygroscopic cryst. Reacts slowly with paraffin hydrocarbons. Dec. >150°. Sol. H_2O, Et_2O; insol. CCl_4, freons. Salts $MAl(ClO_4)_4.2H_2O$ (M = Rb or Cs) also descr.
▷ May explode.
4.5 Hydrate: Colourless hygroscopic cryst.
Hexahydrate: [22993-14-2]. *Hexaaquaaluminium(3+) triperchlorate*
$AlCl_3H_{12}O_{18}$ M 433.4
From hydrated alumina and aq. HCl. Colourless cryst. (H_2O).
Heptahydrate with 4 dioxan: Colourless hygroscopic cryst. (H_2O). Sol. H_2O, MeOH, Me_2CO, EtOAc; spar. sol. Et_2O; insol. C_6H_6, $CHCl_3$, CCl_4.
▷ May explode when dry.
Cl_2O_6 complex:
$AlCl_5O_{18}$ M 492.2
From $AlCl_3$ and Cl_2O_6. Orange v. hygroscopic solid. Sol. SO_2.
▷ May explode with org. liqs.

Hackenberg, E.G. *et al*, *Z. Anorg. Allg. Chem.*, 1939, **243**, 99 (*synth, props*)
Perrier, M. *et al*, *Chem. Ber.*, 1962, **95**, 257 (*synth*)
Bel'kova, M.M. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1966, **40**, 1363 (*thermal dec*)
Movius, W.G. *et al*, *Inorg. Chem.*, 1967, **6**, 847.
Movius, W.G. *et al*, *J. Phys. Chem.*, 1968, **72**, 3063 (*DMF complexes*)
Lamesheva, D.G. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1969, **18**, 1877 (*synth, ir*;hHinton, J.F. *et al*, *Spectrochim. Acta, Part A*, 1969, **25**, 119 (*pmr, dioxan, N-methylacetamide complexes*)
Nikitina, Z.K. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1973, **22**, 723, 971 (*synth, props, ir*)
Nikitina, Z.K. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1974, **22**, 705, 937.
Reuben, Y. *et al*, *J. Phys. Chem.*, 1976, **80**, 2394 (*pmr*)

$AlCl_4^-$ IC-000136

Tetrachloroaluminate(1−)

[17611-22-2]

$[AlCl_4]^-$

M 168.7 (ion)
Species $[M(AlCl_4)_3]^{n-}$, M = Mn, Co or Ni also descr. Species $[AlCl_nBr_{4-n}]^-$ also descr.
Li salt: [14024-11-4]. *Lithium tetrachloroaluminate (LiAlCl4)*
$AlCl_4Li$ M 175.7
Obt. from LiCl and $AlCl_3$. Commercially available. White hygroscopic cryst. (melt). Mp 143.5°. High ionic conductivity in solid: $10^{-4}\ \Omega^{-1}\ m^{-1}$.
Li salt, tris-SO_2 complex: [76229-54-4]. *Tris(sulfur dioxide-O)lithium(1+) tetrachloroaluminate(1−)*
Obt. from $LiCl/AlCl_3/SO_2$. White moisture sensitive cryst. Mp 30°.
Na salt: see *Sodium tetrachloroaluminate*(III) (*$NaAlCl_4$*), *IC-000141*
K salt: [13821-13-1]. *Potassium tetrachloroaluminate ($KAlCl_4$)*
$AlCl_4K$ M 207.8
Obt. from KCl + $AlCl_3$. Colourless moisture sensitive cryst. (melt). Monomers and dimers detected by ms in vapour. $\Delta H^\circ_{f\ 298}$ −1196.6 kJ mol^{-1}; S° 196.6 J K^{-1} mol^{-1}.
Rb salt: [17992-02-8]. *Rubidium tetrachloroaluminate ($RbAlCl_4$)*
$AlCl_4Rb$ M 254.2
Obt. from RbCl + $AlCl_3$. Colourless moisture sensitive cryst. (melt).
Cs salt: see *Caesium tetrachloroaluminate(1−), IC-000137*
Ti(II) *salt:* see *Tetra-μ-chlorobis(dichloroaluminium) titanium*(II), *IC-000280*
Co(II) *salt:* [13820-62-7].
Al_2Cl_8Co M 396.5
Catalyst for polym. of 1,3-butadienes. Blue moisture sensitive needles. Possesses struct. in which $AlCl_4$ tetrahedra and $CoCl_6$ octahedra share corners and edges.
Cu(II) *salt:* see *Copper*(II) *tetrachloroaluminate ($Cu(AlCl_4)_2$), IC-000277*
$Cd_2^{2\oplus}$ salt: see *Cadmium*(I) *tetrachloroaluminate ($Cd_2(AlCl_4)_2$), IC-000275*
$Hg_3^{2\oplus}$ salt: see *Trimercury(2+) bis[tetrachloroaluminate(1−)], IC-000278*
Pd(II) *salt:* see *Tetra-μ-chlorobis(dichloroaluminium) palladium, IC-000279*
Ho salt: see *Hexa-μ-chlorotris(dichloroaluminium)holmium, IC-000346*
H compd.: [29061-29-8]. *Hydrogen tetrachloroaluminate(1−) compd. with diethyl ether (2:3)*
Viscous colourless moisture sensitive oil.
NH_4 salt: [7784-14-7].
$AlCl_4H_4N$ M 186.8
Obt. from NH_4Cl + $AlCl_3$ at 310°. White moisture sensitive solid. Sol. Et_2O. Mp 304°.
Nitrosyl salt: [20137-50-2].
$AlCl_4NO$ M 198.7
Colourless moisture sensitive cryst. Mp 180°.

Friedman, H.L. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 2236 (*synth*)
Baenziger, N.C., *Acta Crystallogr.*, 1951, **4**, 216 (*cryst struct, Na salt*)
Gerding, H. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1956, **75**, 589 (*raman, $NO^\oplus$ salt*)
Ibers, J.A., *Acta Crystallogr.*, 1962, **15**, 967 (*cryst struct, Co salt*)
van der Kamp, L.K. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **361**, 328 (*phase diagram*)
Hasegawa, H. *et al*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
Cyvin, S.J. *et al*, *J. Chem. Phys.*, 1970, **52**, 2776 (*ir, raman*)
Clark, R.J.H. *et al*, *J. Chem. Soc. A*, 1970, 2458 (*ir, H compd*)
Gorenkova, N.V. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 583 (*phase diagram*)
Tiitti, G. *et al*, *Inorg. Chem.*, 1972, **11**, 1439 (*potentiometric data*)
Joosen, D.E.H., *J. Chem. Soc. A*, 1972, 567 (*mixed halide species*)
Pannin, A.A., *J. Electrochem. Soc.*, 1972, **119**, 801 (*electrochem*)
Russell, L.G. *et al*, *J. Electrochem. Soc.*, 1973, **120**, 223 (*thermodyn*)
Rytas, P. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1185 (*raman*)
Morrisey, A.L. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 520 (*synth, vp*)
Merryman, D.J. *et al*, *Inorg. Chem.*, 1974, **13**, 1471 (*mgr*)
Schäfer, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1976, **15**, 713 (*rev*)
Barbier, P. *et al*, *Cryst. Struct. Commun.*, 1976, **5**, 633 (*cryst struct, NO⊕ salt*)
Wepner, W. *et al*, *J. Electrochem. Soc.*, 1977, **124**, 35 (*elec conductivity, Li salt*)
Cisle, R.J. *et al*, *Inorg. Chem.*, 1978, **17**, 2728; 1980, **19**, 2240 (*ir, raman*)
Smyrl, N.R. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1489 (*ir*)
Tarasov, V.P. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1978, **19**, 966 (*Al-27 nmr*)
Kühni, H. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **449**, 145 (*synth, compds with SO_2*)
Perenthaler, E. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **491**, 259 (*Li, Na salts, cryst struct*)
Gesenhues, U. *et al*, *Z. Phys. Chem. (Munich)*, 1982, **132**, 121 (*ms*)
Hussey, C.L., *Adv. Molten Salt Chem.*, 1983, **5**, 185 (*rev*)
Dent, A.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1990, 315 (*complexes*)

$AlCl_4Cs$ IC-000137

Caesium tetrachloroaluminate(1−)

[17992-03-9]

$Cs[AlCl_4]$

M 301.6
$Cs(\mu\text{—}Cl)_3AlCl$ (C_{3v}) in vapour phase. Synth. from CsCl and $AlCl_3$. Colourless moisture-sensitive cryst. (melt). Mp 377°.

Van der Kamp, L.K. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **361**, 328 (*phase diagram*)
Morozov, A.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 520 (*vp*)
Petrov, K.P. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1980, **21**, 310 (*ed*)

$AlCl_4Cu$ IC-000138

Copper tetrachloroaluminate

[27803-79-8]

$CuAlCl_4$

M 232.3
Separates olefins from alkanes; CO from alkanes and arenes, CO_2.

U.S. Pat., 3 754 047, (1973); *CA*, **79**, 104734q.
U.S. Pat., 3 755 487, (1973); *CA*, **79**, 104730k.
Japan. Pat., 78 67 691, (1978); *CA*, **89**, 165629n (*use*)
Japan. Pat., 78 82 695, (1978); *CA*, **89**, 165628m (*use*)

$AlCl_4Ga$ IC-000139

Gallium(*I*) tetrachloroaluminate(*III*)

Aluminium gallium chloride ($AlGaCl_4$)

[11070-76-1]

$Ga[AlCl_4]$

M 238.5
Synth. from Ga, $GaCl_3$ and $AlCl_3$ at 220°. White moisture sensitive solid. Mp 167°.

Peterson, P.J. *et al*, *Aust. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1740, **15**, 1613 (*phase diagram*)
Brinkman, F.J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 667 (*synth, ir, raman*)

IC-000140

$AlCl_3In$

Indium(*I*) tetrachloroaluminate(*III*)

[13933-98-3]

$In[AlCl_4]$

M 283.6
Synth. from $HgCl_2$, Al and In at 325°. May be important in chemical vapour transport. Colourless v. hygroscopic solid. Mp 263°. Reported compd. Al_2Cl_6In not confirmed in later work. With Et_2O gives Indium(*I*) chloride [InCl]. IC-010462 and $[Et_2O.AlCl_3]$

Clark, R.J. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4764 (*synth*)
Larionova, T.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 1131; 1968, **13**, 467; 1968, **14**, 1660 (*phase diagram*)
Brinkman, F.J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 801 (*synth, raman*)
Radloff, P.L. *et al*, *J. Chem. Phys.*, 1980, **72**, 992 (*raman*)
Meyer, G. *et al*, *Z. Naturforsch., B*, 1980, **35**, 117 (*cryst struct*)

IC-000141

$AlCl_4Na$

Sodium tetrachloroaluminate(*III*) ($NaAlCl_4$)

Sodium aluminium chloride (NaAlCl4)
Tetrachloroaluminate(1−), sodium salt, 8CI

[7784-16-9]

$NaAlCl_4$

M 191.7
Synth. by treating a suspension of NaCl in SO_2Cl_2 with $AlCl_3$ in SO_2Cl_2. Catalyst for cracking of hydrocarbons. Pale yellow orthorhombic cryst. Mp 151°. ΔH_f° −1142 kJ mol^{-1}; ΔG_f° −998 kJ mol^{-1}; S° 188 J K^{-1} mol^{-1}. Monomers and dimers detected by ms in vapour.

Baenziger, N.C., *Acta Crystallogr.*, 1951, **4**, 216 (*cryst struct*)
Beattie, I.R. *et al*, *J. Chem. Soc. A*, 1967, 984 (*ir*)
Barbier, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Ser. C*, 1971, **272**, 66 (*synth*)
Schmidt, W. *et al*, *Z. Naturforsch., A*, 1976, **31**, 1354 (*Na-23, Al-27, Cl-35 nmr, mpr*)
Wallart, F. *et al*, *J. Raman Spectrosc.*, 1980, **9**, 33 (*raman, cryst struct*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 90 (*thermodyn data*)

IC-000142

$AlCl_4O_3Re$

Chlorotrioxo(trichloroaluminium)rhenium(*VII*)

Chloro-μ-oxodioxo(trichloroaluminium)rhenium, 10Cl

[71499-76-8]

$ClRe(O)_2{-}O{-}AlCl_3$

M 402.9
Believed to have Re—O—Al bridge. Synth. from ReO_3Cl and $AlCl_3$ in CCl_4. Extremely hygroscopic orange-red cryst. Mp 42°. Ir ν_{Re-O} 949 cm^{-1}.

Lösberg, R. *et al*, *Z. Naturforsch., B*, 1979, **34**, 1040 (*synth, ir*)

IC-000143

$AlCl_4O_{12}S_4^{\ominus}$

Tetrakis(chlorosulfato)aluminate(1−)

Tetrakis(chlorosulfurato-O)aluminate(1−)

$[Al(SO_3Cl)_4]^{\ominus}$

M 489.0 (*ion*)

Na salt: [34460-36-5]
Synth. from $NaAlCl_4$ + SO_3 in liq. SO_2. V. hygroscopic white solid (liq. SO_2); dec. on heating to $NaAl(SO_4)_2$ + $2SO_2Cl_2$. Li and K salts are similar.

Vandorpe, R. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 2878 (*synth, ir, tga*)
Drache, M. *et al*, *Bull. Soc. Chim. Fr.*, 1980, 105 (*reactions*)

IC-000144

$AlCl_6Na_3$

Sodium hexachloroaluminate(*III*) (Na_3AlCl_6)

Trisodium aluminium chloride (Na3AlCl6)
Hexachloroaluminate(3−), trisodium salt, 8CI

[60172-46-5]

Na_3AlCl_6

M 308.6
White solid. Mp 527°. ΔH_f° −2092 kJ mol^{-1}; ΔG_f° −1938 kJ mol^{-1}; S° 377 J K^{-1} mol^{-1}.

Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 92 (*thermodyn data*)

IC-000145

$AlCl_6O_6P_3$

Aluminium dichlorophosphate

Aluminium phosphorodichloridate
Tris(phosphorodichloridato)aluminium

$Al(O_2PCl_2)_3$

M 428.6
Synth. from $AlCl_3$ + Cl_2O/N_2 in $POCl_3$ solv. Colourless, moisture-sensitive cryst. ($POCl_3$). Insol. CCl_4, C_6H_6; spar. sol. Py, $POCl_3$; sol. DMSO, DMF. Mp > 350°.

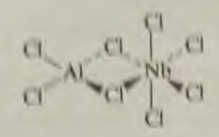
Müller, H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **350**, 231 (*synth, ir*)

IC-000146

$AlCl_6Nb$

Di-μ-chlorotetrachloro(dichloroaluminium)niobium(*V*), 11Cl

[87969-73-1]



M 403.5
The struct. persists in $AlCl_3$ melts and in the vapour phase. Synth. from $AlCl_3$ and $NbCl_5$ at 200° in a sealed ampoule or by heating AlSCl and $NbCl_5$ at the same temp. Mp 139.7°. Corresp. bromide may be similarly obt.

Krebs, B. *et al*, *Inorg. Chem.*, 1984, **23**, 164 (*synth, cryst struct, raman*)

IC-000147

[AlCoFeNi]

Alnico

[8057-41-8]

A family of carbon-free Fe-based alloys containing Al, Ni and Co with some Cu (~3%) and Ti. Alnico V (8 Al, 14 Ni, 24 Co, 3 Cu, 51 Fe) is the most widely used. Produced by casting or by powder metallurgy. Used for permanent magnets.

[12606-66-5]

Berkowitz, A. *et al*, *Magnetism and Metallurgy*, Academic Press, N.Y., 1969, **1**, 473 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **14**, 670.

McCurrie, R.A., *Ferroelectric Materials*, North-Holland, Amsterdam, 1982, **3**, 107 (*rev*)
Lemaire, H., *Powder Metall.*, 1982, **25**, 165 (*rev*)

IC-000148

[AlCr]

Aluminium chromium system

Chromium aluminium

Aluminium chromium **(Al_8Cr_5)**

Al_8Cr_5 M 475.8
Synth. from the elements by rapid quenching of melt from 1215°. Metal.

Brandon, J.K. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1088 (*cryst struct*)

IC-000149

$AlCsF_4$

Caesium tetrafluoroaluminate(1−)

[39211-00-2]

$Cs[AlF_4]$

M 235.8
In solid state, struct. comprises AlF_6 octahedra sharing corners to form 3-fold parallel strands. Cs 8-coord. Monomer $Cs(\mu{-}F)_2AlF_2(C_{2v})$ in vapour. Synth from CsF and AlF_3 at 450° or hydrothermally at 300° and 1600 atm. Transparent moisture sensitive hexagonal plates (melt).

Kolosov, E.N. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1973, **47**, 603 (*ms*)
Piet, F. *et al*, *J. Crystal Growth*, 1979, **47**, 699 (*synth*)
Lösch, R. *et al*, *Z. Naturforsch., B*, 1979, **34**, 131 (*cryst struct*)
Petrov, K.P. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1980, **21**, 310 (*ed*)

IC-000150

$AlCsH_{24}O_{20}S_2$

Aluminium caesium sulfate dodecahydrate

Cesium alum. Cesium aluminium sulfate dodecahydrate. Hexaaquaaluminium(3+) hexaaquacaesium(1+) bis(sulfate)

[7784-17-0]

$[Cs(OH_2)_6][Al(OH_2)_6][SO_4]_2$

M 568.1
In cubic β-alum struct. univalent cation has 12 O neighbours at 355-358 pm: 6 from H_2O and 6 from SO_4. Synth. from Cs_2SO_4 + $Al_2(SO_4)_3$. Colourless cryst. (H_2O). $MeNH_3$ alum is similar.

Lipson, H., *Proc. R. Soc. London, A*, 1935, **148**, 664; **151**, 347 (*cryst struct*)
Inorg. Synth., 1953, **4**, 8 (*synth*)
Haussühl, S., *Z. Kristallogr.*, 1961, **116**, 371 (*props*)
Cromer, D.T. *et al*, *Acta Crystallogr.*, 1966, **21**, 383 (*synth, cryst struct, nd*)
Eysel, H.H. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **424**, 68 (*raman*)
Best, S.P. *et al*, *Inorg. Chem.*, 1980, **19**, 1958 (*ir*)

IC-000151

$AlCsO_6Si_2$

Pollucite

Leucite-Cs

[1308-53-8]

$Cs_{16}[Al_{16}O_{96}Si_{32}]$

M 312.0
Zeolite struct. ANA. A caesium felspathoid. Member of the analcime group with highly distorted channel struct. $Cs[AlSi_2O_{12}]$ and $Cs_{0.35}Al_{0.35}Si_{2.65}O_6$ also descr. Mineral. Hydrothermal synth. from CsOH, $Al(OH)_3$ and silica gel with crystallisation between 160° and 450° or from metakaolinite and aq. CsOH at 80°. Chief ore of caesium. Anhydrous white cryst. (aq. melt). Mp > 1700°. n_D 1.512-1.523.

Nel, H.J., *Am. Mineral.*, 1944, **29**, 443 (*cryst struct*)
Inorg. Synth., 1953, **4**, 8 (*use*)
Barrer, R.M. *et al*, *J. Chem. Soc.*, 1953, 4029; *J. Chem. Soc. A*, 1977, 1020 (*synth*)
Araki, T., *Z. Kristallogr.*, 1980, **152**, 207 (*cryst struct related compd*)
Annehed, H. *et al*, *Z. Kristallogr.*, 1984, **166**, 301 (*cryst struct related compd*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 24.

IC-000152

[AlCu]

Copper-aluminium system

Aluminium copper system. Aluminium bronzes

Many stoichiometries known. As the % Al increases, wear and corrosion resistance increase but ductility decreases.

α-Copper aluminium

α-form
Fcc solid soln. Aluminium bronzes used for carrying corrosive liqs., such as hot brine in salt refineries. Ductile. Forms an eutectic with β phase at 1037° and 8.5% Al.

Copper aluminium **(*3:1*)** [12003-30-4]

β-form
$AlCu_3$ M 217.6
Stronger and harder than α-phase. Dec. on slow cooling to give α + γ_2 at 565° (eutectic), but at normal rates a high proportion of β is retained.

β-form: Stable above 570°. Disordered W type struct.
β_1-form: Exists around ~300° - unstable. $CoAs_3$ type struct.
β'-form: Stable below 300°. Believed to have Cu type struct.

Copper aluminium **(*9:4*)** [12004-92-1]

γ-Copper-aluminium
Al_4Cu_9 M 679.8
Struct. similar to γ-brass.

Copper aluminium **(*2:1*)** [12003-26-8]

$AlCu_2$ M 154.0
hcp struct.

Copper aluminium **(*1:1*)** [12003-21-3]

η-form
AlCu M 90.5
Orthorhombic.

Copper aluminium **(*1:2*)** [12004-15-8]

Al_2Cu M 117.5
Tetragonal metastable states exist. C16 struct. type is stable form. This consists of 5-connected nets of Al atoms, with Cu atoms between layers.

Bradley, A.J. *et al*, *J. Inst. Met.*, 1933, **51**, 131 (*struct, β-form; Al_2Cu*)
Wassermann, G. *et al*, *Metallwiss., Metalltech.*, 1934, **13**, 133 (*struct, β-form*)
Dowson, A.G., *J. Inst. Met.*, 1937, **61**, 197 (*α-form, struct*)
Bradley, A.J. *et al*, *J. Inst. Met.*, 1938, **63**, 149 (*struct, γ-form, η-form*)
Nelson, J.B. *et al*, *Proc. Phys. Soc., London*, 1945, **57**, 160 (*struct, γ-form*)
Axon, H.J. *et al*, *Proc. R. Soc. London, A*, 1955, **193**, 1 (*struct, Al_2Cu*)
Duval, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Ser. C*, 1968, **267**, 388 (*struct, β-form*)
Rabkin, D. *et al*, *Poroshk. Metall. (Kiev)*, 1970, **10**, 101 (*synth, phys props, β-form, Cu_3Al*)

Yamamoto, K.A. *et al*, *J. Phys. Colloq.*, 1971, **32** (*x-ray spec.*, Cs_2AlF_5)
Yamamoto, K.A. *et al*, *Phys. Status Solidi B*, 1971, **43**, 319 (*x-ray spec.*, Cs_3AlF_6)
Fedorov, M. *et al*, *J. Less-Common Met.*, 1972, **29**, 133 (*struct.*, *o-form*)
Siukhov, D.S. *et al*, *Fiz. Met. Metalloved.*, 1975, **39**, 715 (*magnetism*, Cs_2AlF_5, *o-form*)
Brugger, K. *et al*, *Helv. Phys. Acta*, 1974, **47**, 321 (*x-ray*, *o-form*)
Arnberg, L. *et al*, *Acta Crystallogr., Sect. A*, 1978, **34**, 474 (*struct.*, Cs_2AlF_5)
Zeigler, H. *et al*, *Aluminium* (Duesseldorf), 1979, **55**, 332 (*phys props.*, Cs_2AlF_5)
Anisimov, V.I. *et al*, *Solid State Commun.*, 1980, **36**, 769 (*qes*)
Macedonio, C. *et al*, *Thin Solid Films*, 1981, **81**, 71 (*conductivity*, *γ-form*, Al_2Cs)
Tepping, R.L. *et al*, *Can. J. Spectrosc.*, 1983, **28**, 87 (*ps*, *h-form*, Al_2Cs)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct., props*)

IC-000153

AlF

Aluminium(*I*) fluoride (AlF)

[13595-52-9]

AlF

M 45.9
Detected in graphite furnace from solns. cont. Al^{III} and $F^{\ominus}$. Al—F 165.4 pm. Used in detection of sub-nanogram quantities of $F^{\ominus}$. Not isol. ΔH_f° AlF (g) −265.3 kJ mol^{-1}; S° 215 J K^{-1} mol^{-1}.

Lide, D.R. *et al*, *J. Chem. Phys.*, 1965, **42**, 1013 (*microwave*)
Hoell, J. *et al*, *Z. Naturforsch., B*, 1970, **25**, 901 (*synth, microwave*)
Rosenwaks, S., *J. Chem. Phys.*, 1976, **65**, 3668 (*chemiluminescence*)
Tsunoda, K. *et al*, *Anal. Chem.*, 1977, **49**, 2035; **51**, 2059 (*use*)
Chiba, K. *et al*, *Anal. Chem.*, 1980, **52**, 1582 (*use*)
Tsuneda, K. *et al*, *Spectrochim. Acta, Part B*, 1980, **35**, 715 (*at.*)

IC-000154

AlF_3

Aluminium(*III*) fluoride (AlF_3)

Aluminium trifluoride

[7784-18-1]

AlF_3

M 83.9
Has LaF_3 struct. in solid state. Mainly monomeric in vapour, with small amounts of dimer. Constit. of electrolyte in aluminium smelting. Also in ceramics, glass, enamels. With KHF_2 reagent for prepn. of fluorohydrins. Commercially available. Colourless cryst. Spar. sol. H_2O; insol. org. solvs. Subl. 1270°, ε 4.9; n_D 1.382. $\Delta H_{f\,298}^\circ$ −1510.4 kJ mol^{-1}; S° 66.5 J K^{-1} mol^{-1}.

▷ BD0725000.

Trihydrate: [15098-87-0].
α-Form from HF and Al; β-form from aq. AlF_3 at 100°. Colourless cryst. (H_2O).
Nonahydrate: [15098-89-2].
Colourless cryst. (H_2O).

Porter, R.F. *et al*, *J. Chem. Phys.*, 1960, **33**, 858 (*ms, thermodyn*)
Gabuda, S.P. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1962, **10**, 225 (*pmr, F-19 nmr*)
McCory, L.D. *et al*, *J. Phys. Chem.*, 1963, **67**, 1086 (*ir*)
Matijević, E. *et al*, *J. Phys. Chem.*, 1969, **73**, 564 (*soly*)
Foster, P.A., *J. Am. Ceram. Soc.*, 1970, **53**, 598 (*phase diagram*)
Murat, M. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 3101 (*hydrate*)
McGuire, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Nefedov, V.I. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **18**, 490 (*hydrate*)
Nicholls, C.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 901 (*x-ray emission*)
Yang, Y.S. *et al*, *J. Mol. Spectrosc.*, 1975, **54**, 39 (*ir*)
Dulepov, E.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1976, **21**, 1780 (*synth, props, ir*)
Nirsha, B.M. *et al*, *Zh. Obshch. Khim.*, 1979, **49**, 1690 (*hydrate*)
Ichihara, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 1848 (*synth, use*)

IC-000155

$AlF_4^{\ominus}$

Tetrafluoroaluminate(1 −)

[21340-02-3]

$[AlF_4]^{\ominus}$

M 102.9 (ion)
Li salt: see *Lithium tetrafluoroaluminate(1 −)*, *IC-000157*
Na salt: see *Sodium tetrafluoroaluminate(1 −)*, *IC-000158*
K salt: see *Potassium tetrafluoroaluminate(1 −)*, *IC-000156*
Rb salt: see *Rubidium tetrafluoroaluminate(1 −)*, *IC-000159*
Cs salt: see *Caesium tetrafluoroaluminate(1 −)*, *IC-000149*
Brosset, C., *Z. Anorg. Allg. Chem.*, 1938, **239**, 301 (*synth, powder struct*)
Krasnov, K.S., *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1972, **46**, 1237; 1977, **51**, 1769; 1978, **52**, 1783 (*theory*)
Soga, T., *J. Chem. Phys.*, 1974, **61**, 1990 (*ir*)
Huglen, R. *et al*, *Z. Naturforsch., A*, 1979, **34**, 1118 (*ir*)

AlF_4K **IC-000156**

Potassium tetrafluoroaluminate(1 −)

[14484-69-6]

$K[AlF_4]$

M 142.0
In solid state, AlF_6 octahedra share corners to give layers with K between. Exists as $K(\mu\text{—}F)_2AlF_2$ molecule in vapour. Synth. from KF and AlF_3 at 600° or hydrothermally at 300° and 1600 atm. Hygroscopic colourless plates.

Brosset, C., *Z. Anorg. Allg. Chem.*, 1938, **239**, 301 (*powder struct*)
Soga, T. *et al*, *J. Chem. Phys.*, 1974, **61**, 1990 (*synth, ir*)
Kolosov, E.N. *et al*, *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1975, **49**, 476 (*ms*)
Thompson, W.T. *et al*, *Can. J. Chem.*, 1976, **54**, 3342 (*phase diagram*)
Vajda, E. *et al*, *Inorg. Chim. Acta*, 1977, **25**, L143 (*ed*)
Plet, F. *et al*, *J. Crystal Growth*, 1979, **47**, 699 (*synth*)
Wanklyn, B.M. *et al*, *J. Mater. Sci.*, 1979, **14**, 1447 (*synth*)
Nouet, J. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 32 (*cryst struct*)

AlF_4Li **IC-000157**

Lithium tetrafluoroaluminate(1 −)

[15138-76-8]

$Li[AlF_4]$

M 109.9
Synth from $LiAlH_4$ and F_2/He. Light grey hygroscopic powder.

Porter, R.F. *et al*, *J. Chem. Phys.*, 1960, **33**, 858 (*ms*)
McCory, L.D. *et al*, *J. Phys. Chem.*, 1963, **67**, 1086 (*ir*)
Garton, G. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 2461 (*powder data*)
Cyvin, S.J. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **380**, 212; *J. Phys. Chem.*, 1971, **75**, 2609 (*ir, thermodyn data*)
Snelson, A. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **390**, 316 (*thermodyn data*)
Lagow, R.J. *et al*, *Inorg. Chim. Acta*, 1974, **10**, 9 (*synth, ms, powder struct*)

Dewing, E.W., *J. Electrochem. Soc.*, 1976, **123**, 1289; *Metall. Trans. B*, 1980, **11**, 245 (*thermodyn data*)
Di, T. *et al*, *Mater. Res. Bull.*, 1981, **16**, 1281 (*electrical conductivity*)

AlF_4Na **IC-000158**

Sodium tetrafluoroaluminate(1 −)

[13821-15-3]

$Na[AlF_4]$

M 125.9
Monomers, $Na(\mu\text{—}F)_2AlF_2$, and dimers detected in vapour. Synth. from NaF and AlF_3. Solid by rapid condensation of vapour. Slow cooling gives $Na_5Al_3F_{14}$ and AlF_3. White hygroscopic solid.

Howard, E.H. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2041 (*synth*)
Ginsberg, H. *et al*, *Z. Elektrochem.*, 1957, **61**, 315 (*phase diagram*)
McCory, L.D. *et al*, *J. Phys. Chem.*, 1963, **67**, 1086 (*ir*)
Rolin, M. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 891 (*vp*)
Garton, G. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 2461 (*powder struct*)
Sidorov, L.N., *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1967, **173**, 370 (*ms*)
Spiridonov, V.P. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 332 (*ed*)
Bondam, J., *Acta Chem. Scand.*, 1971, **25**, 3271 (*ir*)
Cyvin, S.J. *et al*, *J. Phys. Chem.*, 1971, **75**, 2609 (*ir*)
Dewing, E.W., *Metall. Trans.*, 1971, **2**, 495 (*thermodyn data*)
Snelson, A. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **390**, 316 (*thermodyn data*)
Holm, J.L., *Acta Chem. Scand.*, 1973, **27**, 371, 1410 (*props*)

AlF_4Rb **IC-000159**

Rubidium tetrafluoroaluminate(1 −)

[14484-70-9]

$Rb[AlF_4]$

M 188.4
AlF_6 octahedra share 4 corners to give layers or chains. Several modifications descr. Synth from RbF and AlF_3 at 600° or hydrothermally at 300° and 1600 atm. White hygroscopic solid.

Brosset, C., *Z. Anorg. Allg. Chem.*, 1938, **239**, 301 (*powder struct*)
Sogar, T. *et al*, *J. Chem. Phys.*, 1974, **61**, 1990 (*synth, ir*)
Plet, F. *et al*, *J. Crystal Growth*, 1979, **47**, 699 (*synth*)
Fourquet, J.L. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1997 (*cryst struct*)
Couzi, M. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1983, **87**, 232 (*ir*)

AlF_4Tl **IC-000160**

Thallium(*I*) tetrafluoroaluminate(1 −)

[33897-69-7]

$Tl[AlF_4]$

M 307.3
4 Vertices of AlF_6 octahedra are shared to give layer $Tl[AlF_4]$ struct. (primitive tetrag.). Hydrothermal synth. using AlF_3 and aq. 5*M* TlF soln. in HF (300°, 2 atm.); from $Al(OH)_3$ and TlF in liq. HF. White brittle plates. Spar. sol. H_2O; insol. alcohols, ethers. No hydrate formed.

▷ Toxic.

Brosset, C., *Z. Anorg. Allg. Chem.*, 1937, **235**, 139; **239**, 301 (*synth, cryst struct*)
Feather, D. *et al*, *J. Phys. Chem.*, 1973, **77**, 1599.
Plet, F. *et al*, *J. Crystal Growth*, 1979, **47**, 699 (*synth*)
Fourquet, J.L. *et al*, *Rev. Chim. Miner.*, 1979, **16**, 490 (*struct*)
Wells, A.F., *Structural Inorg. Chem.*, 5th Ed, Clarendon Press, Oxford, 1984, 469.

$AlF_5H_4Hg_2O_2$ **IC-000161**

Disquadimercury(2+) pentafluoroaluminate(2 −)

[80420-63-9]

$[Hg_2(H_2O)_2]_n(AlF_5)_n$

M 559.1
AlF_6 octahedra share two corners to give infinite chains. Synth. from aq. Hg_2F_2 and AlF_3 in aq. HF at 150° and 150 atm. Colourless needles (HF).

Fourquet, J.L. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 2136 (*synth, cryst struct*)

AlF_5Mn **IC-000162**

Aluminium manganese(*II*) fluoride ($AlMnF_5$)

Aluminium manganese pentafluoride, 10CI

[12421-24-8]

$MnAlF_5$

M 176.9
MnF_6 and AlF_6 octahedra present; Mn—F 209, 206 pm. Synth. by heating equimolar amounts of AlF_3 and MnF_2 at 700° under Ar.

Cousseins, J.C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 717 (*synth*)
Rimsky, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **270**, 407 (*cryst struct*)
Tressaud, A. *et al*, *Mater. Res. Bull.*, 1973, **8**, 565 (*synth, magnetism*)
Wintenberger, M. *et al*, *Solid State Commun.*, 1975, **17**, 185 (*magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1977, **C4**, 243 (*rev, bibl*)

$AlF_6^{3\ominus}$ **IC-000163**

Hexafluoroaluminate(3 −)

[21340-03-4]

$[AlF_6]^{3\ominus}$ (O_h)

M 140.9 (ion)
Li salt: see *Lithium hexafluoroaluminate*(III) (Li_3AlF_6), *IC-000165*
Na salt: see *Sodium hexafluoroaluminate* (Na_3AlF_6), *IC-000166*
Tri-K salt: see *Potassium hexafluoroaluminate*(III) (K_3AlF_6), *IC-000164*
Tri-Rb salt: [13844-92-3]. *Rubidium hexafluoroaluminate* (Rb_3AlF_6). *Trirubidium hexafluoroaluminate*
AlF_6Rb_3 M 397.3
Obt. from RbF and AlF_3. White solid (melt). Mp 905°.
Tri-Cs salt: [13844-93-4]. *Caesium hexafluoroaluminate* (Cs_3AlF_6). *Tricaesium hexafluoroaluminate*
$AlCs_3F_6$ M 539.6
Obt. from CsF and AlF_3. White solid (melt). Mp 723°.
Tri-NH_4 salt: [7784-19-2].
Obt. from H_3AlF_6 and NH_4OH. White hygroscopic powder. Insol. EtOH. Possible percursor for synth. of AlN.

▷ BD0050000.

Bode, H. *et al*, *Z. Anorg. Allg. Chem.*, 1957, **290**, 1 (*rev*)
Holm, J.L., *Acta Chem. Scand.*, 1965, **19**, 261 (*eqa, synth*)
Thompson, W.T. *et al*, *Can. J. Chem.*, 1976, **54**, 3342 (*phase diagram, K salt*)

Grimmer, A.R. *et al*, *Z. Chem.*, 1982, **22**, 43 (*Al-27, F-19 nmr*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 108 (*thermodyn data*)

IC-000164

AlF_3K_3

Potassium hexafluoroaluminate(*III*) (K_3AlF_6)

Tripotassium aluminium fluoride (K_3AlF_6)

Hexafluoroaluminate(3–), tripotassium salt

[13775-52-5]

K_3AlF_6

M 258.2

Tetragonal cryolite struct. Converts to a second tetragonal form at 143° and undergoes a tetragonal to cubic transition at 327°. Synth. by melting together AlF_3 and KF in a 2:1 ratio. Used in brazing fluxes, also as a fireproofing agent for polycarbonates. Commercially available. Colourless cryst. Mp 1040°, ΔH_f° –3326 kJ mol^{-1}; ΔG_f° –3163 kJ mol^{-1}; S° 285 J K^{-1} mol^{-1}.

Steward, E.G. *et al*, *Acta Crystallogr.*, 1953, **6**, 49 (*polymorph*)
Holm, J.L., *Acta Chem. Scand.*, 1965, **19**, 26 (*struct, synth*)
Alcaraz, S., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **260**, 1977 (*synth*)
Rouldid, M.J., *Spectrochim. Acta, Part A*, 1973, **29**, 1923 (*ir, raman*)

IC-000165

AlF_6Li_3

Lithium hexafluoroaluminate(*III*) (Li_3AlF_6), 8CI

Trilithium aluminium fluoride. Hexafluoroaluminate(3–) trilithium salt, 9CI

[13821-29-0]

Li_3AlF_6

M 161.7

Struct. related to cryolite. Several modifications descr. AlF_6 octahedra linked by Li, each with 6 F neighbours. Prepd. by melting together LiF and AlF_3 at 780°. Colourless orthorhombic cryst. Undergoes orthorhombic to tetragonal transition at 510° and tetragonal to cubic transition at 597°. Mp 785°. ΔH_f° –3384 kJ mol^{-1}; ΔG_f° –3224 kJ mol^{-1}; S° 187.9 JK^{-1} mol^{-1}.

Rolin, M. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 891 (*synth*)
Garton, G. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 2466 (*powder struct*)
Burns, J.H. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 225 (*cryst struct*)
Holm, J. *et al*, *Acta Chem. Scand.*, 1969, **23**, 1065 (*polymorphs*)
Arthurs, S.D. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 3435 (*synth*)
Dewing, E.W., *Metall. Trans. B*, 1980, **11**, 245 (*thermodyn*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 109 (*thermochem data*)

IC-000166

AlF_6Na_3

Sodium hexafluoroaluminate (Na_3AlF_6)

Trisodium hexafluoroaluminate(3–)

Hexafluoroaluminate(3–), trisodium salt, 8CI

[13775-53-6]

$Na_3[AlF_6]$

M 209.9

Made industrially from HF, Al_2O_3, NaOH. Alternatively manuf. either by reaction of aq. HBF_4 with mixtures of Na_2CO_3 and $Al(OH)_3$ or by treatment of aq. $AlCl_3$ with HF in presence or NaF or NaCl. Commercially available. Electrolyte in Hall-Héroult process for Al manuf. Component of fluxes, esp. for welding steels. Cryst. monoclinic colourless when pure. Undergoes monoclinic to cubic transition at 563°. Spar. sol. H_2O. Mp 1012°. $AlF_5^{2\ominus}$, $AlF_4^\ominus$ and $F^\ominus$ ions detected in melt. Elec. cond. 4 x 10^{-4} $\Omega^{-1}m^{-1}$ (solid); 282 $\Omega^{-1}m^{-1}$ (melt). ΔH_f° –3317 kJ mol^{-1}; ΔG_f° –3152 kJ mol^{-1}; S° 238 J K^{-1} mol^{-1}.

▷ Corrosive, toxic.

Mineral-form [15096-52-3]

Cryolite

Structural prototype, consists of $Na^\oplus$ cations and discrete $AlF_6^{3\ominus}$ anions. Closely related is Cryolithionite which is $Li_3Na_3Al_2F_{12}$. Occur. esp. in Greenland. Aluminium ore. White or discoloured brittle solid.

▷ WA9625000.

Brosset, C., *Z. Anorg. Allg. Chem.*, 1938, **238**, 201 (*rel compd*)
Naray-Szabo, I. *et al*, *Z. Kristallogr.*, 1938, **99**, 27 (*cryst struct*)
Steward, E.G. *et al*, *Acta Crystallogr.*, 1953, **6**, 49 (*phase trans*)
Ginsberg, H. *et al*, *Z. Elektrochem.*, 1957, **61**, 315 (*phase diagram*)
Foster, P.A., *J. Am. Ceram. Soc.*, 1960, **43**, 66; 1968, **51**, 107; 1970, **53**, 598; 1975, **58**, 288 (*phase diagram, elect cond*)
Meyers, M.D. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 5027 (*ir*)
Rolin, M. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 891 (*vp*)
Foster, P.A., *J. Chem. Eng. Data*, 1964, **9**, 200 (*phase diagram*)
Dewing, E.W., *J. Electrochem. Soc.*, 1970, **117**, 780 (*phase diagram*)
Bondam, J., *Acta Chem. Scand.*, 1971, **25**, 3271 (*ir*)
McGuire, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Nicholls, C.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 901 (*x-ray emission*)
Courbion, G. *et al*, *Mater. Res. Bull.*, 1974, **9**, 425 (*rel compds*)
Grimmer, A.R. *et al*, *Z. Chem.*, 1982, **22**, 43 (*F-19 nmr, Al-27 nmr*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 112 (*thermochem data*)
Burkin, A.R. Ed., *Prod. Alum. and Alumina, 1987*, Wiley, 1987, 85.
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3141B (*haz*)

IC-000167

$AlF_6O_6P_3$

Aluminium difluorophosphate

Aluminium phosphorodifluoridate.

Tris(phosphorodifluoridato)aluminium

$Al(PO_2F_2)_3$

M 329.8

Synth. from $AlCl_3$ and $HOP(O)F_2$. White powder. Insol. C_6H_6, CCl_4, CH_2Cl_2. Mp >300°.

Shihada, A.F. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **466**, 139 (*synth, ir*)

IC-000168

$AlFe_{0.5}H_2Mg_{2.75}O_{12}Si_3$

Vermiculite

[1318-00-9]

$Mg_{0.25}(H_2O)_4[(Mg_{2.5}Fe_{0.5})(AlSi_3)O_{10}(OH)_2]$

M 400.0

Struct. has Pyrophyllite, IC-000289 layers with Al replacing some Si in tetrahedral sites, $Mg^{2\oplus}$ and $Fe^{3\oplus}$ in octahedral sites, and interlayer hydrated $Mg^{2\oplus}$. Widely distributed mineral. Insulator and fireproof filler in construction industry. Widely used industrial absorbent and catalyst. Whitish brown solid. Cation exchange capacity 1.0-1.5 eq kg^{-1}.

Mathieson, A.McL., *Am. Mineral.*, 1954, **39**, 231 (*cryst struct*)
Van Olpen, H., *Introduction to Clay Colloid Chemistry*, 2nd Ed., Wiley, N.Y., 1977.

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 239; **6**, 191, 202; **15**, 416; **21**, 283.
Sanz, J. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 4790 (*Al-27, Si-29 nmr*)
Kinsey, R.A. *et al*, *Am. Mineral.*, 1985, **70**, 537 (*Al-27, Si-29 nmr*)

[AlFe] **IC-000169**

Iron aluminium system

Aluminium iron

Alloy.

Iron aluminum *(3:1)* [12003-42-8]

$AlFe_3$ M 194.5

Parent of the Fe_3Al structural type. Based on bcc lattice; subject to order-disorder transformations. Used in various engineering applications; on aluminized carbon steel. Compds. of stoichiometries 1:1, 2:1, 3:1, 4:1, 5:1, 5:2, 6:1 and 13:4 also known.

Koster, W. *et al*, *Z. Metallk.*, 1980, **71**, 765 (*phase diagram*)
Min, B.I. *et al*, *J. Magn. Magn. Mater.*, 1986, **54**, 1091 (*electronic struct, magnetism*)
Skjerpe, P., *J. Microsc. (Oxford)*, 1987, **148**, 33 (*struct*)

$AlFe_6H_{13}Mn_5NaO_{44}Si_{12}$ **IC-000170**

Howieite, 9CI

[67034-78-0]

$Na(Fe^{II},Fe^{III},Mn,Al,Mg)_{12}[Si_6O_{17}]_2(O,OH)_{10}$

M 1713.8

Mineral. A chain silicate. Also formulated as $Na(Fe^{II},Mn)_{10}(Fe^{III},Al)_2Si_{12}O_{31}(OH)_{13}$. Occurs in metamorphic rocks of the Franciscan formation in California and at other locations. Dark green to black anorthic blades.

Wenk, H.R., *Am. Mineral.*, 1974, **59**, 86 (*cryst struct*)
Wood, R.M., *Mineral. Mag.*, 1979, **43**, 363 (*mineral*)

$AlGaI_4$ **IC-000171**

Gallium(*I*) tetraiodoaluminate(*III*)

Aluminium gallium iodide ($AlGaI_4$)

$Ga[AlI_4]$

M 604.3

Synth. from Ga, GaI_3 and AlI_3 at 200°. Pale yellow moisture-sensitive solid. Mp 180°. Forms continuous solid solns. with Gallium(*I*) tetraiodogallate(*III*), IC-019097.

Fedorov, P.I. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **23**, 1376 (*synth, phase diagram*)

$AlGeNaO_4$ **IC-000172**

Aluminium germanium sodium oxide ($AlGeNaO_4$)

[12251-11-5]

$Na[AlGeO_4]$

M 186.5

Isostructural with $CaFe_2O_4$: has chains of double edge-sharing MO_6 octahedra linked by shared corners. Na ions in inter-chain tunnels; Al and Ge randomly distributed in octahedral M sites. Synth. from melt at 1.2 × 10^5 atm. and 900°. It is unclear whether compd. from hydrothermal synth. is same. White cryst. (melt). n_D 1.815.

Reid, A.F. *et al*, *Acta Crystallogr.*, 1967, **23**, 736 (*cryst struct*)
Reid, A.F. *et al*, *Inorg. Chem.*, 1968, **7**, 112 (*synth, propn*)
Uvarova, T.G. *et al*, *Kristallografiya*, 1976, **21**, 866; *C.A.*, **85**, 169751 (*synth*)

$AlHO_2$ **IC-000173**

Aluminium hydroxide oxide (Al(OH)O)

Basic aluminium oxide

[24623-77-6]

AlO(OH)

M 59.9

White solid. Sol. hot NaOH.

▷ BD0950000.

α-form [14457-84-2]

Diaspore

Struct. has AlO_6 octahedra with shared edges and corners, some linked by H bonds. Mineral from Paraguay and Pennsylvania. White or off-white cryst.

γ-form [1318-23-6]

Boehmite

AlO_6 octahedra share edges to form double layers joined by H bonds. From gelatinous $Al(OH)_3.xH_2O$ at 350° and 300 atm. Mineral. White solid.

Hoppe, W., *Z. Kristallogr.*, 1940, **103**, 73; 1942, **104**, 11 (*diaspore, cryst struct*)
Thibon, H. *et al*, *Bull. Soc. Chim. Fr.*, 1951, 384 (*synth*)
Milligan, W.O. *et al*, *J. Phys. Chem.*, 1956, **60**, 273 (*boehmite, cryst struct*)
Busing, W.R. *et al*, *Acta Crystallogr.*, 1958, **11**, 798 (*diaspore, cryst struct, nd*)
Papeé, D. *et al*, *Bull. Soc. Chim. Fr.*, 1958, 1301 (*synth*)
Holm, C.H. *et al*, *J. Phys. Chem.*, 1958, **62**, 992 (*boehmite, pmr*)
Kroon, D.J. *et al*, *Nature (London)*, 1959, **183**, 944 (*boehmite, pmr*)
Beretka, J. *et al*, *J. Chem. Soc. A*, 1967, 2106 (*boehmite, synth*)
Sato, T., *Z. Anorg. Allg. Chem.*, 1972, **391**, 69, 167 (*synth*)
Russell, J.D. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 1151 (*boehmite, ir*)
Slade, R.C.T. *et al*, *J. Solid State Chem.*, 1980, **32**, 119 (*pmr*)
Farmer, V.C., *Spectrochim. Acta, Part A*, 1980, **36**, 585 (*boehmite, ir, raman*)
Kiss, A.B. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 653 (*boehmite, ir, raman*)

$AlHO_{34}P_4U_8$ **IC-000174**

Sabugalite

[12042-24-9]

$AlH(UO_2)_4(PO_4)_4$

M 1487.9

Formulated as $(HAl)_{0.5}(UO_2PO_4)_2$ with 16 or 10 H_2O. Mineral, member of autunite group. Occurs at various sites in USA, Europe and Brazil. Bright yellow cryst. + $16H_2O$.

Walenta, K., *Chem. Erde.*, 1965, **24**, 254
Vochten, R. *et al*, *Phys. Chem. Miner.*, 1983, **9**, 23 (*synth, ips, dta, cryst struct*)
Cejca, J. *et al*, *Phys. Chem. Miner.*, 1984, **11**, 172 (*ir*)
Weigel, F., *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, **1**, 372 (*propn*)

$AlH_2KMg_3O_{12}Si_3$ **IC-000175**

Phlogopite

[61076-94-6]

$K[Mg_3(OH)_2Si_3AlO_{10}]$

M 417.2

Mica with layers of $Mg(O,OH)_6$ octahedra between $(Si,Al)O_4$ tetrahedra. $K^\oplus$ between layers. Mineral in basic

... magnesium synthetic material from oxide melts. Used as ... insulators in universal equipment, gaskets, perpendicular to ... cover, occurring in beds. Distinctive vitreous ... Fluorophlogopite, in which F replaces OH also dimor. Li may replace Mg.

[12510-38-0]

Fukuda, H. *et al.*, *Kyoto Gemmologic.* 1980, **30**, 838 (cryst struct, ...)
Iler, Colloid Chem. Technol., 2nd Ed., Wiley, N.Y., 1979 ...
1984, 13, 550, 14, 419 (cryst) ...
Ivano, T. *et al.*, *J. Am. Ceram. Soc.*, 1984, **100**, 6700 (-0.27 nm/..., 20 nm/...)
Mingi, M. *et al.*, *Phys. Chem.*, 1984, **88**, 1518 (20-29 nm/..., 20 nm/...)
Krauss, E.A. *et al.*, *Am. Mineral.*, 1985, **70**, 547 (-0.27, 20-30 nm/...)

$AlH_2Mg_2Na_2O_{10}Si_5$

Arfvedsonite

[12169-16-1]

$Na_2Mg_4(AlSi_5O_{22})(OH)_2$

M 603.8

Amphibole. Struct. with double chains. Much isomorphous replacement occurs e.g. Fe for Al in natural forms. Synth. from SiO_2, $Al(OH)_3$, $MgCl_2$, NaCl at 450-550° and 0.4-1.4 x 10^{-3} atm. Widely distributed mineral. Fibrous white cryst. Specimens com. Fe are coloured greenish-black, black.

Denisova, N.D., *Geol. Geofiz.*, 1988, 119; *CA*, 1970, **72**, 34209 (synth)
Hawthorne, F.C., *Can. Mineral.*, 1978, **16**, 345; *C.A.*, **89**, 152234 (cryst struct)
Lapidus, I.L., *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1980, 254, 986 (pr)
Kazmin, V.N. *et al.*, *Geokhimiya*, 1982, 1523 (ir)

$AlH_2NaO_4Si_2$

Analcime

Analcite (improper)

[1318-18-1]

$Na_{16}[Al_{16}Si_{32}O_{96}].16H_2O$

M 220.1

Zeolite struct. ANA composed of $(AlSi\text{-}O)_6$ and $(Al_2Si\text{-}O)_{12}$ rings with irregular channels formed by highly distorted $(AlSi\text{-}O)_6$ rings. Formed hydrothermally from component oxides. Mineral found in both igneous and sedimentary rocks in USA, Norway, Germany, Australia and elsewhere. White cryst. (aq. melt). n_D 1.486.

Barrer, R.M. *et al.*, *J. Chem. Soc.*, 1952, 1561; 1959, 195 (synth)
Barrer, R.M. *et al.*, *J. Chem. Soc.*, 1953, 4029, 4035 (synth, K, Rb, Tl, Cs forms)
Barrer, R.M. *et al.*, *J. Chem. Soc.*, 1956, 2882 (synth, K form)
Barrer, R.M. *et al.*, *J. Chem. Soc.*, 1961, 983; 1964, 485 (synth, Ca, Sr forms)
Ferraris, G. *et al.*, *Z. Kristallogr.*, 1972, **135**, 240 (cryst struct ref)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, 1974, 209 (props)
Mazzi, F. *et al.*, *Am. Mineral.*, 1978, **63**, 448 (cryst struct)
Lippmaa, E. *et al.*, *J. Am. Chem. Soc.*, 1981, **103**, 4992; 1986, **108**, 1730 (Si-29 nmr, Al-27 nmr)
Barrer, R.M. *et al.*, *Hydrothermal Chemistry of Silicates*, Academic Press, 1982, 240.
Artioli, G. *et al.*, *Acta Crystallogr., Sect. C*, 1984, **40**, 214 (P-substr compd)
Meier, W.M. *et al.*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 24.

AlH_3

Aluminium(III) hydride (AlH_3)

Alane

[7784-21-6]

AlH_3

M 30.0

Solid state struct. comprises 3-D network of Al—H—Al with Al octahedrally coord. Synth. from $LiAlH_4$ and $AlCl_3$ in Et_2O or $LiAlH_4$ and H_2SO_4 in THF. Commercially available. White amorph. or microcryst. air and moisture sensitive solid. Usually made in THF or Et_2O and used *in situ*. Several solid forms descr. Solids $AlH_3.nEt_2O$, n = 0.3-3 obt. from Et_2O. Sol. Et_2O, THF.

▷ BD0930000.

Me_3N complex: see *Trihydro(trimethylamine)aluminium, IC-000375*

Et_3N complex: [12076-08-3].
$C_6H_{18}AlN$ M 131.1
Synth. from $[Et_3NH]Cl$ and $LiAlH_4$. White air- and moisture-sensitive liq. Mp 13-15°.

Finholt, A.E. *et al.*, *J. Am. Chem. Soc.*, 1947, **69**, 1199 (*synth*)
Dautel, R. *et al.*, *Z. Elektrochem.*, 1960, **64**, 1234 (*ir*)
Rosinski, H. *et al.*, *Z. Phys. Chem. (Munich)*, 1963, **36**, 26 (*ir*)
Brown, H.C. *et al.*, *J. Am. Chem. Soc.*, 1966, **88**, 1464 (*synth*)
Turley, J.W. *et al.*, *Inorg. Chem.*, 1969, **8**, 18 (*cryst struct, nd*)
Cucinella, S. *et al.*, *Inorg. Chim. Acta Rev.*, 1970, 51 (*rev*)
Semenenko, K.N. *et al.*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 949, 1104 (*ir*)
Zakharkin, L.I. *et al.*, *Zh. Obshch. Khim.*, 1971, **41**, 577 (*synth, complexes*)
Inorg. Synth., 1973, **14**, 47 (*synth*)
Ashby, E.C. *et al.*, *J. Am. Chem. Soc.*, 1973, **95**, 6485 (*synth*)
Boiko, G.N. *et al.*, *Usp. Khim.*, 1975, **44**, 3 (*rev*)
Brower, F.M. *et al.*, *J. Am. Chem. Soc.*, 1976, **98**, 2450 (*synth, props*)

AlH_3O_3

Aluminium hydroxide ($Al(OH)_3$)

[21645-51-2]

$Al(OH)_3$

M 78.0

Commercially available. White solid (H_2O). Proc. insol. H_2O; sol. conc. aq. acids and alkalis. Forms gel on prolonged contact with H_2O.

▷ BD0940000.

Gel: [1330-44-5]. *Algedrate, USAN, INN. Aluminium hydroxide hydrate. W4600*
Antacid.

Mineral-form [14762-49-3]
Gibbsite. Hydragillite
Double layer of close packed OH of held by H bonds with Al in $\frac{2}{3}$ octahedral holes. Widespread mineral occurs as an alteration product of aluminium bearing minerals (Norway). Colourless hexagonal platelets.

Mineral-form [20257-20-9]
Bayerite
Layer struct. with O approx. hcp and Al octahedrally coord. Synth. from aq. $AlCl_3$ and $[NH_4]OH$ at pH 8. Mineral occurs in sedimentary rock at sites in Israel and Britain. White powder, colourless monoclinic cryst.

Mineral-form [13840-05-6]
Nordstrandite

Double layers of AlO_6 octahedra with shared edges and corners linked by H bonds. Obt. by cryst. of $Al(OH)_3$ using $(CH_2OH)_2$ or $(CH_2NMe_2)_2$. Mineral found at many locations. Colourless, beige, pink and pale green cryst.

Mineral-form
Dayleite
Mineral found at sites in Canada. Creamy or bluish white triclinic cryst.

Thibon, H. *et al.*, *Bull. Soc. Chim. Fr.*, 1951, 384 (*props*)
Calvet, E. *et al.*, *Bull. Soc. Chim. Fr.*, 1953, 99 (*props*)
Brown, J.F. *et al.*, *J. Chem. Soc.*, 1953, 84 (*gibbsite, thermal dec*)
van Nordstrand, R.A. *et al.*, *Nature (London)*, 1956, **177**, 713 (*nordstrandite*)
Papeé, D. *et al.*, *Bull. Soc. Chim. Fr.*, 1958, 1301 (*props*)
Kroon, D.J. *et al.*, *Nature (London)*, 1959, **183**, 944 (*gibbsite, bayerite, pmr*)
Wall, J.R.D. *et al.*, *Nature (London)*, 1962, **196**, 264 (*nordstrandite*)
Hathaway, J.C. *et al.*, *Nature (London)*, 1962, **196**, 265 (*nordstrandite*)
Hauschild, U., *Z. Anorg. Allg. Chem.*, 1963, **324**, 15 (*synth, ir, powder struct, props*)
Lippens, C. *et al.*, *Acta Crystallogr.*, 1964, **17**, 1312 (*phase trans*)
Beretka, J. *et al.*, *J. Chem. Soc. A*, 1967, 2106 (*bayerite, gibbsite, synth, props*)
Rothbauer, R. *et al.*, *Z. Kristallogr.*, 1967, **125**, 317 (*bayerite, cryst struct, nd*)
Bosmans, H.J. *et al.*, *Acta Crystallogr., Sect. B*, 1970, **26**, 649 (*nordstrandite, cryst struct*)
Sato, T., *Z. Anorg. Allg. Chem.*, 1972, **391**, 69 (*synth*)
Singh, S.S., *Soil Sci. Am. Proc.*, 1974, **38**, 415 (*soly, gibbsite*)
Saalfield, H.L. *et al.*, *Z. Kristallogr.*, 1974, **139**, 129 (*gibbsite, cryst struct*)
Smyshiyaev, S.I. *et al.*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 528 (*thermodyn data*)
Chang, B.-T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 1960 (*gibbsite, thermodyn data*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, **28/29**, 12340.
Aluminium Chems. Sci. and Tech. Handbook, (Hart, D.Le.R., Ed.), Amer. Ceram. Soc., 1990.

$AlH_3O_8P_2$

Aluminium phosphate ($AlH_3(PO_4)_2$)

Aluminium phosphate (1:2). Aluminium trihydrogen bisphosphate

[13967-89-0]

$AlH_3(PO_4)_2$

M 219.9

Several hydrates descr. From $(NH_4)_2HPO_4$ + $Al_2(SO_4)_3$ followed by dehydration at 200°. Constit. of many commercial binders and adhesives. White cryst. On heating, undergoes a complex series of reactions.

Monohydrate: [66906-02-3].
From Al_2O_3, H_3PO_4, H_2O at 100-120°. White solid.

Trihydrate: [39611-87-5].
From Al_2O_3, H_3PO_4 and H_2O at 25°. White solid (H_2O).

d'Yvoire, F., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1958, **247**, 297.
Martin, R. *et al.*, *Bull. Soc. Chim. Fr.*, 1960, 851 (*phase diagram*)
d'Yvoire, F., *Bull. Soc. Chim. Fr.*, 1961, 2283 (*synth, powder struct*)
Morris, J.H. *et al.*, *Chem. Soc. Rev.*, 1977, **6**, 173 (*hydrates, use*)

$AlH_4^{\ominus}$

Tetrahydroaluminate(1−)

Aluminohydride

[19469-81-9]

$[AlH_4]^{\ominus}$ (T_d)

M 31.0 (ion)

Li salt: see *Lithium aluminium hydride, IC-000183*

Na salt: [13770-96-2]. *Sodium tetrahydroaluminate. Aluminium sodium hydride ($AlNaH_4$). Lithium alanate*
AlH_4Na M 54.0
From Na, Al and H_2 in THF at 150° and 140 atm. White v. moisture sensitive solid. Insol. Et_2O; sol. THF, diglyme. Mp 174° (185-190°). Dec. rapidly at 185°. $\Delta H_{f\ 298}^{\circ}$ −113 kJ mol^{-1}.
▷ BD0180000.

K salt: [16903-34-7]. *Potassium tetrahydroaluminate. Aluminium potassium hydride*
AlH_4K M 70.1
From K, Al and H_2 in diglyme at 150° and 140 atm. White v. hygroscopic solid. Insol. Et_2O, C_6H_6; sol. THF, diglyme. ΔH_f° −166.5 kJ mol^{-1}.

Cs salt: [16961-92-5]. *Caesium tetrahydroaluminate. Aluminium caesium hydride*
$AlCsH_4$ M 163.9
From Cs, Al and H_2 at 130° and 300 atm. White v. moisture sensitive solid. Sol. diglyme; spar. sol. toluene. Mp 310-314°. ΔH_f° −166.5 kJ mol^{-1}.

Me_4N salt: [16903-67-6].
$C_4H_{16}AlN$ M 105.1
Synth. from Me_4NBr and $LiAlH_4$. White air and moisture sensitive powder. Insol. Et_2O, THF (Et_4N salt more sol.). Dec. without melting at 170°.

Finholt, A.E. *et al.*, *J. Am. Chem. Soc.*, 1947, **69**, 1199 (*synth*)
Lippincott, E.R., *J. Chem. Phys.*, 1949, **17**, 1351 (*ir, raman*)
Gaylord, N.G., *Reductions with Complex Metal Halides*, Interscience, N.Y., 1956 (*rev*)
Ashby, E.C., *Inorg. Chem.*, 1963, **2**, 499; 1972, **11**, 1230 (*synth, tga*)
Ehrlich, R. *et al.*, *Inorg. Chem.*, 1965, **4**, 758 (*synth*)
Ashby, E.C., *Adv. Inorg. Chem. Radiochem.*, 1966, **8**, 283 (*rev*)
Sklar, N. *et al.*, *Inorg. Chem.*, 1967, **6**, 669 (*cryst struct*)
McCarty, M. *et al.*, *J. Phys. Chem.*, 1968, **72**, 4009 (*dec*)
Haraguchi, H. *et al.*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
Gorin, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1970, 3790 (*powder struct*)
Titov, L.V. *et al.*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1507 (*synth, alkylammonium deriv, ir, tga*)
Anderson, J.W. *et al.*, *J. Chem. Soc. A*, 1971, 2246 (*reactions*)
Crea, J. *et al.*, *Inorg. Chem.*, 1972, **11**, 1131 (*reactions*)
McGuire, G.E. *et al.*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Ashby, E.C. *et al.*, *J. Am. Chem. Soc.*, 1973, **95**, 2823; 1975, **97**, 3158 (*conduct*)
Shirk, A.E. *et al.*, *J. Am. Chem. Soc.*, 1973, **95**, 5904 (*ir, raman*)
Dymova, T.N. *et al.*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1974, **216**, 87 (*tga*)
Semenenko, K.N. *et al.*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 338 (*synth*)
Kuznetsov, V.A. *et al.*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 669 (*synth, tga*)
Hermanek, S., *Chem. Ind. (London)*, 1975, 42 (*Al-27 nmr*)
Ashby, E.C., *J. Org. Chem.*, 1976, **41**, 2890 (*use*)
Pizey, J.S., *Lithium Aluminium Hydride*, Horwood-Wiley, 1977 (*rev*)
Lithium Aluminium Hydride, Properties, Handling, Applications, Chemetall Frankfurt, 1984 (*props, use, haz*)
Tarasov, V.P. *et al.*, *Koord. Khim.*, 1985, **11**, 1626 (*Al-27 nmr*)
Singalova, S.V. *et al.*, *Zh. Obshch. Khim.*, 1989, **59**, 348 (*ir*)

AlH_4LaNi_4

Aluminium lanthanum nickel hydride ($AlLaNi_4H_4$)

$AlLaNi_4H_4$

M 404.6

Has potential applications in H_2-storage; chemical heat pump. Light to dark grey powder. Loses H_2 on heating.

▷ May be pyrophoric in air.

Green, D.M. *et al*, *Solar Energy*, 1978, **19**, 153 (*use*)
Mendelsohn, M.H. *et al*, *Inorg. Chem.*, 1979, **18**, 3343.
Inorg. Synth., 1983, **22**, 96 (*synth*)

IC-000183

AlH_4Li
Lithium aluminium hydride
Lithium tetrahydroaluminate(III). Tetrahydroaluminate, lithium salt, 8CI. Lithium aluminohydride. Lithal. Lithium alanate
[16853-85-3]

$LiAlH_4$

M 37.9
Prepd. by reaction of LiH with $AlCl_3$ or $AlBr_3$ in Et_2O or from $NaAlH_4$ and LiCl in Et_2O. Commercially available as solid or in soln. in Et_2O (1.0 *M*), diglyme (0.5 *M*) and THF (1.0 *M*). Versatile reducing agent. Polym. catalyst. Moisture sensitive white monoclinic cryst. Reacts violently with H_2O. Dec. on heating to form LiH, Al and H_2. Sol. Et_2O (39g per 100 cm^3), THF (15g per 100g); spar. sol. hydrocarbons. ΔH_f° –117 kJ mol^{-1}; ΔG_f° –48 kJ mol^{-1}; S° 87.9 J K^{-1} mol^{-1}.

▷ Flammable, corrosive. May catch fire in air without warning. BD0100000.

Deuterio derivs.: [14128-54-2]. *Lithium aluminium deuteride (LiAlD$_4$). Deuterated lithium aluminium hydride. Lithium tetrahydroaluminate - d_4. Tetrahydroaluminate - d_4, lithium salt, 8CI*

AlD_4Li M 41.9
Prepd. from $AlBr_3/Et_2O$ + LiD/Et_2O or from Li, Al and D_2 at 150°, 15 atm. Commercially available. Reducing agent for producing deuterated organics. V. moisture sensitive white cryst. Sol. Et_2O; spar. sol. hydrocarbons. Dec. at 98°.

▷ Produces HD on reacting violently with H_2O.

Ashby, E.C., *Adv. Inorg. Chem. Radiochem.*, 1966, **8**, 283 (*rev*)
Carvill, M. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 2295 (*synth, LiAlD$_4$*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 581; 1969, **2**, 342; 1972, **3**, 176; 1974, **4**, 291; 1975, **5**, 382; 1977, **6**, 325; 1979, **7**, 196; 1980, **8**, 286; 1981, **9**, 274; 1982, **10**, 236; 1984, **11**, 289; 1986, **12**, 272.
Sklar, N. *et al*, *Inorg. Chem.*, 1967, **6**, 669 (*cryst struct*)
Pyykko, P. *et al*, *Chem. Phys. Lett.*, 1968, **2**, 297 (*D nmr*)
Shirk, A.E. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 5904 (*ir, raman*)
Hermanek, S. *et al*, *Chem. Ind. (London)*, 1975, 42 (*Al-27 nmr, LiAlD$_4$*)
Horne, D.A., *J. Am. Chem. Soc.*, 1980, **102**, 6011 (*gmr, Li-7 nmr*)
Nöth, H., *Z. Naturforsch., B*, 1980, **35**, 119; 1981, **36**, 31 (*Li-7 nmr, Al-27 nmr*)
Tarasov, V.P. *et al*, *Koord. Khim.*, 1981, **7**, 674 (*Al-27 nmr, LiAlD$_4$*)
Baker, R.W., *Report MLM-3193 (1984)*, 1984; *CA*, 1985, **102**, 186094 (*LiAlD$_4$, uses*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 122 (*thermochem data*)
Bastide, J.P. *et al*, *Mater. Res. Bull.*, 1985, **20**, 999 (*LiAlD$_4$, struct, polymorph*)
Burtaux, J.C. *et al*, *Mater. Res. Bull.*, 1985, **20**, 1147 (*LiAlD$_4$, raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2149D, 2149B, 2149C.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2132.

$AlH_4O_4^\ominus$ IC-000184
Aluminate ($Al(OH)_4^\ominus$), 9CI
Tetrahydroxyaluminate(1–)
[14485-39-3]

$[Al(OH)_4]^\ominus$

M 95.0 (ion)
Species obs. in basic solns. containing Al.
Haraguchi, H. *et al*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
Yoshio, M. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 1365 (*polym*)
Moolenaar, R.J. *et al*, *J. Phys. Chem.*, 1970, **74**, 3629 (*raman, Al-27 nmr*)
Mesmer, R.E. *et al*, *Inorg. Chem.*, 1971, **10**, 2290 (*thermodyn*)
Volokhov, Yu.A. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1975, **16**, 930 (*pmr*)
Dovbysh, N.G. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1978, **52**, 1578 (*pmr*)
Miller, A.G. *et al*, *Anal. Chem.*, 1980, **52**, 807 (*raman*)
Tracey, A.S. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 4901 (*Al-27 nmr*)

IC-000185

$AlH_5O_9P_2$
Aluminium phosphate ($Al(H_2PO_4)(HPO_4).H_2O$)
Aluminium trihydrogen bis(phosphate) hydrate

$Al(H_2PO_4)(HPO_4).H_2O$

M 237.9
$AlO_5(OH_2)$ octahedra share vertices with $PO_2(OH)_2$ and $PO_3(OH)$ tetrahedra to form 2-dimensional frameworks linked by H-bonds. Synth. from aq. soln. containing Al:PO_4 1:3 at 110°. Colourless hexagonal plates (H_2O).
Brosheer, J.C. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 5951 (*phase diagram*)
Jameson, R.F. *et al*, *J. Chem. Soc.*, 1954, 4013 (*phase diagram*)
Kniep, R. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1047 (*synth, cryst struct*)

IC-000186

$AlH_6^{3\ominus}$
Hexahydroaluminate(3–)

$[AlH_6]^{3\ominus}$

M 33.0 (ion)
Salts formed as intermeds. in dec. of $MAlH_4$. Derivs. of several other metals also descr.

Tri-Li salt: [16941-14-3].
AlH_6Li_3 M 53.8
Synth. from $LiAlH_4$ and BuLi. White air- and moisture-sensitive microcryst. solid (hexane/Et_2O). Insol. hydrocarbons, Et_2O. Mp 210° dec. Ir ν_{Al-H} 1720 cm^{-1}.

Tri-Na salt: [17069-12-4].
AlH_6Na_3 M 101.9
Synth. from Na, Al, Et_3Al, in toluene with 300 atm. H_2; or from $NaAlH_4$ and $NaAlH_2(OCH_2CH_2NMe_2)_2$ in C_6H_6. White air- and moisture-sensitive solid. Insol. hydrocarbons, Et_2O.

Tri-K salt: [17083-63-5].
AlH_6K_3 M 150.3
Obt. from Al, K and H_2 (300 atm.). Grey air- and moisture-sensitive solid. Insol. hydrocarbons, Et_2O.

Tri-Cs salt: [53436-80-9].
$AlCs_3H_6$ M 431.7
Obt. from dec. of $CsAlH_4$ at 350°.

Tri-Cu(I) salt: [62126-19-6].
$AlCu_3H_6$ M 223.6
Not isol. Detected in mixtures of $LiAlH_4$ and CuI used as reagent for conjugate reduction α,β-enones.

Ashby, E.C. *et al*, *Inorg. Chem.*, 1966, **5**, 1615; 1969, **8**, 2468 (*synth*)
Ehrlich, R. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 858 (*synth*)
Dilts, J.A. *et al*, *Inorg. Chem.*, 1972, **11**, 1230 (*iga*)
Macháček, J. *et al*, *Collect. Czech. Chem. Commun.*, 1973, **38**, 343; **43**, 1441 (*synth, reactions, Na salt*)
Dymova, T.N. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1974, **216**, 87 (*iga*)

Kuznetsov, V.A., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 669 (*iga*)
Ashby, E.C. *et al*, *Inorg. Chem.*, 1977, **16**, 1437 (*Cu salt*)

AlH_6N_3 IC-000187
Aluminium amide ($Al(NH_2)_3$)
Triaminoalane
[73052-67-2]

$Al(NH_2)_3$

M 75.0
Synth. from AlH_3 + $3NH_3$. On heating gives AlN. Moisture-sensitive white powder. Loses NH_3 above –30°. Insol. Et_2O, other org. solvs.
Wiberg, E. *et al*, *Z. Naturforsch., B*, 1955, **10**, 231 (*synth*)
Wiberg, E. *et al*, *Hydrides of the Elements of the Main Groups I-IV*, Elsevier, Amsterdam, 1971 (*synth*)
Maya, L., *Adv. Ceram. Mater.*, 1986, **1**, 150 (*use*)

$AlH_6O_{12}P_3$ IC-000188
Aluminium phosphate ($Al(H_2PO_4)_3$)
Aluminium phosphate (1:3), 9CI, 8CI. Aluminium tris(dihydrogen phosphate)
[13530-50-2]

$Al(H_2PO_4)_3$

M 317.9
Synth. from $Al(OH)_3$ + H_3PO_4; Al + H_3PO_4; Al_2O_3 + H_3PO_4 at <300°. Employed in binders eg. for glazes; metal coatings; dental cements. V. hygroscopic colourless hexagonal prisms. Mp 243°. When heated forms condensed Al phosphates via an amorphous form produced at 230-290°. Many similar compds. $Al(H_2PO_4)_x(HPO_4)_y(H_2O)_z$ descr.

Dihydrate: [124606-61-7].
Synth. from Al_2O_3—P_2O_5—H_2O system.

(1)-form
Rhombohedral cell. Isolated AlO_6 octahedra are stacked with corner-sharing PO_4 tetrahedra, and the columns are linked by H bonds. V. hygroscopic prisms. Mp 243°. Undergoes phase transition at 60° with proton reorientation.

(2)-form
Trigonal unit cell. Hygroscopic colourless cryst.

Jameson, R.F. *et al*, *J. Chem. Soc.*, 1954, 4013 (*synth*)
D'Yvoire, F.B., *Bull. Soc. Chim. Fr.*, 1961, 2227 (*props*)
Christyakova, A.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 536; *Inorg. Materials (Engl. Transl.)*, 1969, **5**, 449 (*props*)
Morris, J.H. *et al*, *Chem. Soc. Rev.*, 1977, **6**, 173 (*rev*)
Kniep, R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1978, **17**, 272 (*synth, cryst struct*)
Kniep, R. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1047; 1979, **34**, 750; 1980, **35**, 403 (*rel compds*)
Brodalla, D. *et al*, *Z. Naturforsch., B*, 1981, **36**, 907 (*cryst struct*)
Bobrov, B.S. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1983, **56**, 1463; *J. Appl. Chem. USSR (Engl. Transl.)*, 1983, **56**, 1370 (*synth*)
Lyutsko, V.A. *et al*, *Zh. Neorg. Khim.*, 1989, **34**, 2024; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1989, **34**, 1152 (*synth, ir*)

$AlH_8N_4^\ominus$ IC-000189
Tetrakis(amido)aluminate(1–)
Tetraaminoaluminate(1–). Tetrakis(amino)aluminate(1–)

$[Al(NH_2)_4]^\ominus$ (T_d)

M 91.0 (ion)
Related ions e.g. $[Al_2(NH_2)_5]^{2\ominus}$ also descr.

Li salt: [67849-02-9].
Translucent v. hygroscopic microcryst. Dec. >95°.

Na salt: [16456-83-0].
AlH_8N_4Na M 114.0
From Na, Al in liq. NH_3. V. hygroscopic white cryst. (liq. NH_3). Loses NH_3 on heating.

K salt: [18131-29-8].
V. hygroscopic white cryst. (liq. NH_3). Several crystalline forms descr.

Cs salt: [21790-63-6].
V. hygroscopic white cryst. (liq. NH_3).

Ca salt (2:1) monoammoniate: [39914-88-0].
V. hygroscopic white cryst. (liq. NH_3).

Rouxel, J. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1966, **262**, 1070 (*synth*)
Brec, R. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **264**, 512; *Bull. Soc. Chim. Fr.*, 1968, 2721 (*synth*)
Palvadeau, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **269**, 126; 1972, **275**, 881 (*cryst struct, ir*)
Brec, R. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **270**, 491; 1972, **274**, 266 (*cryst struct, ir*)
Molinié, P. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 925 (*cryst struct*)

$AlH_8P_4^\ominus$ IC-000190
Tetrakis(phosphido)aluminate(1–)
Tetraphosphinoaluminate(1–)

$[Al(PH_2)_4]^\ominus$

M 158.9 (ion)

Li salt: [25248-80-0].
From $LiAlH_4$ and PH_3. Made in diglyme, used *in situ*.

Na salt: [34807-16-4].
AlH_8NaP_4 M 181.9
From $AlCl_3$ and $NaPH_2$. Made in diglyme, used *in situ*.

Finholt, A.E. *et al*, *Inorg. Chem.*, 1963, **2**, 504 (*synth, use*)
Norman, A.D. *et al*, *Inorg. Chem.*, 1970, **9**, 870; 1975, **14**, 1095 (*synth, use*)
Fritz, G. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **385**, 243; 1974, **407**, 287 (*synth, use, pmr, P-31 nmr*)
Demuth, R. *et al*, *J. Fluorine Chem.*, 1973, **2**, 269 (*use*)
Inorg. Synth., 1974, **15**, 178 (*synth, use*)

$AlH_{12}O_6^{3\oplus}$ IC-000191
Hexaaquaaluminium(3+)
[15453-67-5]

$[Al(OH_2)_6]^{3\oplus}$

M 135.0 (ion)
Species in acid solns. cont. Al.

Dilodate, nitrate: [57682-96-9].
Synth. from $Al(NO_3)_3$ + HIO_3 (1:2). Colourless platy cryst. (H_2O). Formulated as $[Al(OH_2)_6][IO_3]_2[NO_3]$.

H compd, complex with iodic acid: [62671-54-9].
Synth. from $Al(NO_3)_3$ + HIO_3 (1:6). Colourless cryst. (H_2O). Formulated as $[Al(OH_2)_6][IO_3]_2[HI_2O_8]HIO_3$. See also Aluminium iodate ($Al(IO_3)_3$), 1C-000197.

Aveston, J. *et al*, *J. Chem. Soc.*, 1965, 4438 (*hydrol*)
Movious, W.G. *et al*, *Inorg. Chem.*, 1967, **6**, 847 (*pmr*)
Supran, L.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 832 (*pmr*)
Fratiello, A. *et al*, *J. Chem. Phys.*, 1968, **48**, 3705 (*pmr*)
Haraguchi, H. *et al*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
Kálmán, E. *et al*, *Z. Phys. Chem. (Leipzig)*, 1970, **244**, 106; 245, 425 (*props*)
Mesmer, R.E. *et al*, *Inorg. Chem.*, 1971, **10**, 2290 (*hydrol*)
Akitt, J.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 604; 1973, 42; 1981, 1606 (*Al-27 nmr, pmr*)

Latysheva, V.A., *Russ. J. Phys. Chem. (Engl. Transl.)*, 1972, **46**, 767 (*ir*)
Cradwick, P.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1926; 1977, 146 (*cryst struct*)
Cammidi, R. *et al*, *J. Chem. Phys.*, 1978, **71**, 2473 (*x-ray diffr data*)
Best, S.P. *et al*, *Inorg. Chem.*, 1980, **19**, 1958 (*ir*)
Tracey, A.S. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 4901 (*Al-27 nmr*)
Saito, K. *et al*, *Polyhedron*, 1990, **9**, 215 (*kinetics*)

IC-000192

AlIO

Aluminium iodide oxide (AlIO)
Aluminium(III) oxide iodide
[13596-13-9]

AlIO

M 169.8
Struct. has $(AlO)_n$ and I layers. Synth. from $AlI_3 + As_2O_3$ at 250°. Colourless v. hygroscopic solid. Insol. org. solvs.

Hagenmuller, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1961, **253**, 667.
Hagenmuller, P. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **323**, 1 (*synth, powder struct*)
Batsanov, S.S. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1968, **9**, 282 (*rev*)

IC-000193

AlIS

Aluminium(*III*) iodide sulfide (AlIS)

AlIS

M 185.9
Synth. from $Al_2S_3 + AlI_3$ at 300°. V. hygroscopic white needles (melt). Insol. Et_2O, Me_2CO, C_6H_6, THF.

Hagenmuller, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1961, **253**, 667 (*synth*)
Hagenmuller, P. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **323**, 1 (*synth, powder struct*)
Lin Zhengyan, *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 67 (*synth, raman, ir*)

IC-000194

AlISe

Aluminium iodide selenide (AlISe)
Aluminium(III) selenide iodide
[29758-56-3]

AlISe

M 232.8
Synth. from Al_2Se_3 and AlI_3 at 350°. V. hygroscopic white powder. Insol. Et_2O, C_6H_6, Me_2CO, THF, CS_2, CCl_4.

Palvadeau, P. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 2698 (*synth, powder struct, props*)
Lin Zhengyan, *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 67 (*synth, ir, raman*)

IC-000195

AlITe

Aluminium iodide telluride (AlITe)
Aluminium(III) telluride iodide

AlITe

M 281.4
Synth. from Al, I_2 and Al_2Te_3. Extremely hygroscopic creamy white solid (melt). Insol. Et_2O, EtOH, Me_2CO, C_6H_6, dioxan, $CHCl_3$, CS_2, CCl_4.

Rouxel, J. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2044 (*synth, props*)

AlI_3

Aluminium(*III*) iodide (AlI_3)
Aluminium triiodide
[7784-23-8]

AlI_3

M 407.6
In cryst., AlI_4 tetrahedra share corners to give chains as in SO_3. Lewis acid. Friedel-Crafts catalyst. Commercially available. White moisture sensitive cryst. Mp 179-189°. ΔH_f° AlI_3(s) −280.4 kJ mol^{-1}, S°_{298} 219.9 J K^{-1} mol^{-1}. Many complexes descr.
▷ Reacts violently with H_2O.

Tris-Py complex:
$C_{15}H_{15}AlI_3N_3$ M 644.9
White moisture-sensitive solid. Sol. MeOH; spar. sol. most org. solvs. Mp 195-198° dec.

Inorg. Synth., 1953, **4**, 117; 1980, **20**, 82 (*synth, complexes*)
Segel, S.L., *J. Chem. Phys.*, 1956, **25**, 578 (*nqr*)
O'Reilly, D.E., *J. Chem. Phys.*, 1960, **32**, 1007 (*Al-27 nmr*)
Greenwood, N.N. *et al*, *Friedel-Crafts Rel. Reacts.*, (Ed. Olah, G.A.), Wiley, N.Y., 1963, **1**, 569 (*uses*)
Beattie, I.R. *et al*, *J. Chem. Soc. A*, 1968, 813; 1969, 2655 (*ir, raman*)
O'Brien, J.F. *et al*, *J. Phys. Chem.*, 1970, **74**, 743 (*complexes*)
McGuire, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Anthoney, M.E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 659 (*thermodyn*)
Kniep, R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 386.
Dalibart, M. *et al*, *Coord. Chem. Rev.*, 1986, **74**, 1 (*complexes*)

IC-000197

AlI_3O_9

Aluminium iodate ($Al(IO_3)_3$)

$Al(IO_3)_3$

M 551.6
Obt. from $[Al(OH_2)_6][IO_3][HI_2O_6].HIO_3$ at 340°. Forms double salt $[Al(OH_2)_6][IO_3]_2[NO_3]$.

Endrédy, A., *Z. Anorg. Allg. Chem.*, 1934, **217**, 53 (*synth, hydrate*)
Matějček, J. *et al*, *Collect. Czech. Chem. Commun.*, 1966, **31**, 190 (*synth*)
Cradwick, P.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1926; 1977, 146 (*synth, cryst struct double salt*)
Ivanov-Emin, B.N. *et al*, *Koord. Khim.*, 1979, **5**, 515 (*synth*)

IC-000198

AlI_3O_{12}

Aluminium periodate ($Al(IO_4)_3$)

$Al(IO_4)_3$

M 599.6
Double salt with $LiClO_4$ used in sepn. of Li from Na.

Dodecahydrate:
$AlH_{24}I_3O_{24}$ M 815.8
From $Al(NO_3)_3$ and $Na_2H_3IO_6$. Colourless cryst. (H_2O).

Ferrari, A. *et al*, *Gazz. Chim. Ital.*, 1961, **91**, 77 (*synth*)
Matějček, J. *et al*, *Collect. Czech. Chem. Commun.*, 1966, **31**, 190 (*synth, props*)

IC-000199

$AlI_4^{\ominus}$

Tetraiodoaluminate(1−)
[22602-43-3]

$[AlI_4]^{\ominus}$ (T_d)

M 534.6 (ion)
Li salt: [17992-04-0]. *Lithium tetraiodoaluminate* ($LiAlI_4$)
AlI_4Li M 541.5

Synth. from AlI_3 and LiI. White moisture-sensitive solid (melt). Mp 237°.
Na salt: [18007-74-4]. *Sodium tetraiodoaluminate* ($NaAlI_4$)
AlI_4Na M 557.5
Synth. from AlI_3 and NaI. Colourless moisture-sensitive solid (melt). Mp 220°.
K salt: [17992-05-1]. *Potassium tetraiodoaluminate* ($KAlI_4$)
AlI_4K M 573.6
Synth. from AlI_3 and KI. Colourless moisture-sensitive solid (melt). Mp 210°.
Rb salt: [18007-75-5]. *Rubidium tetraiodoaluminate* ($RbAlI_4$)
AlI_4Rb M 620.0
Synth. from AlI_3 and RbI. Colourless moisture-sensitive solid (melt). Mp 205°.
Cs salt: [18007-76-6]. *Caesium tetraiodoaluminate* ($CsAlI_4$)
$AlCsI_4$ M 667.5
Synth. from AlI_3 and CsI. Colourless moisture-sensitive solid (melt). Mp 250°. $Cs[Al_2I_7]$ also descr.
Tetraiodophosphonium salt: [86086-64-8].
Tetraiodophosphorus(1+) tetraiodoaluminate(1−)
AlI_8P M 1073.1
Synth. from $PI_3 + I_2 + AlI_3$. Dark red extremely moisture-sensitive cryst. (CS_2). Mp 110°. cf. AlI_9P_2.
Pentaiododiphosphorus(1+) salt:
AlI_9P_2 M 1231.0
Synth. from $AlI_3 + PI_3$ in CS_2. Dark brown moisture-sensitive cryst. Mp 127-130°.

Baudler, M. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **329**, 3 (*synth, $P_2I_5^{\oplus}$ salt*)
Boef, G. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **353**, 93 (*phase diagram*)
Mikheeva, V.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1012 (*phase diagram*)
Kinsella, E. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 2139 (*ir*)
Arkhipov, S.M. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 419 (*phase diagram*)
Begun, G.M. *et al*, *Inorg. Chem.*, 1971, **10**, 886 (*raman*)
Okuda, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 3136 (*nqr*)
Pohl, S., *Z. Anorg. Allg. Chem.*, 1983, **498**, 15, 20 (*cryst struct, PI_4 and P_2I_5 salts*)

$AlInS_3$

IC-000200

Aluminium indium sulfide ($AlInS_3$)
Aluminium indium trisulfide
[72840-32-5]

$AlInS_3$

M 238.0
Struct. comprises network of AlS_4 tetrahedra sharing corners with InS_5 trigonal bipyramids. Synth. from $Al_2S_3 + In_2S_3$ by chem. vap. transport with I_2 at 800° to 750°. Light yellow hexagonal pyramids.

Schulte-Kellinghaus, M. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 3016 (*cryst struct*)

$AlKO_2$

IC-000201

Aluminium potassium oxide ($AlKO_2$)
Potassium aluminium oxide ($KAlO_2$). Potassium aluminate ($KAlO_2$)
[12003-63-3]

$KAlO_2$

M 98.0
Has $NaFeO_2$ struct. Synth. from Al_2O_3 and K_2CO_3 at 1200°. White solid. ΔH_f° −1141 kJ mol^{-1}. K_3AlO_3 and K_5AlO_4 also descr.

Gevorkyan, S.V. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1972, **17**, 808 (*reactions*)
Bon, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **278**, 785 (*related compds*)
Eliezer, I. *et al*, *J. Phys. Chem.*, 1978, **25**, 2688 (*thermodyn data*)
Brumakin, E.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 1868 (*synth, powder struct*)
Müller, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1277 (*Al-27 nmr*)

$AlKO_6Si_2$

IC-000202

Leucite
[1302-34-7]

$K_{16}[Al_{16}Si_{32}O_{96}]$

M 218.2
Zeolite struct. ANA. Isotypic with Analcime, IC-000177 but with no water in framework. Felspathoid of analcime group. Mineral, occurs in potassium-rich basic lavas. Found in USA, Canada, Germany, Zaire, Australia and elsewhere. Several modifications described including tetragonal low temp. and cubic high temp. forms.

Barrer, R.M., *J. Chem. Soc.*, 1953, 1879 (*ion exchange*)
Peacor, D.R., *Z. Kristallogr.*, 1968, **127**, 213 (*cryst struct*)
Mazzi, F., *Am. Mineral.*, 1976, **61**, 108 (*cryst struct, low temp form*)
Engelhardt, G. *et al*, *High Resolution Solid State NMR of Silicates and Zeolites*, Wiley, 1987, 242 (*Si-29 nmr*)

$AlKO_8S_2$

IC-000203

Aluminium potassium sulfate ($AlK(SO_4)_2$)
Sulfuric acid, aluminium potassium salt (2:1:1), 8CI. Anhydrous alum
[10043-67-1]

$KAl(SO_4)_2$

M 258.2
Struct. comprises alternate layers of six coordinate $Al^{3\oplus}$ and $K^{\oplus}$ with $SO_4^{2\ominus}$ between. Synth. by dehydration of the alum. Commercially available. Coagulating agent for rubber; also used in deodorants and waste water treatment. Colourless hexagonal plates (H_2SO_4). Sol. H_2O (7.74 g per 100 cm^3 at 30°); insol. EtOH. Corresp. $NH_4^{\oplus}$, $Rb^{\oplus}$, $Cs^{\oplus}$ salts also descr. ΔH_f° −2470 kJ mol^{-1}; ΔG_f° −2240 kJ mol^{-1}; S° 205 J K^{-1} mol^{-1}.
Dodecahydrate: [7784-24-9]. *Potassium alum. Kalinite. Hexaaquaaluminium(3+) hexaaquapotassium(1+) bis(sulfate). α-Alum*
$AlH_{24}KO_{20}S_2$ M 474.3
May be synth. from Al_2O_3, $H_2SO_4 + K_2SO_4$. Mineral. Mordant. Used in H_2O purif., paper sizing, dressing skins. Commercially available. Colourless cryst. (H_2O). Sol. H_2O (11 g per 100 cm^3 at 20°); insol. EtOH, Me_2CO. Mp 105°. Dec. on heating (−$9H_2O$ at 64.5°, −$12H_2O$ at 200°).
▷ WS5690000.

[14635-80-4]

Lipson, H., *Proc. R. Soc. London, A*, 1935, **148**, 664; **151**, 347 (*cryst struct, dodecahydrate*)
Klug, H.P. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 1492 (*dodecahydrate, cryst struct*)
Young, F.E., *J. Am. Chem. Soc.*, 1945, **67**, 257 (*synth, thermodyn props*)
Palmer, W.G., *Experimental Inorganic Chemistry*, CUP, 1959, 216 (*synth, dodecahydrate*)
Burns, G., *Phys. Rev.*, 1961, **123**, 64 (*dodecahydrate, pmr*)
Tret'yakov, Yu.D. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1961, 859 (*phase diagram*)
Haussühl, S., *Z. Kristallogr.*, 1961, **116**, 371 (*props*)

Franks, W. *et al*, *Acta Crystallogr., Sect. B*, 1965, **19**, 870 (*anhydrous, cryst struct*)
Crowe, D.T. *et al*, *Acta Crystallogr.*, 1967, **22**, 800 (*nd, dodecahydrate*)
Vandorpe, B. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **266**, 379 (*related compds*)
Mazeli, J.-M. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 98 (*synth, cryst struct*)
Rems, P. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 33 (*ir*)
Gal, S., *Therm. Anal., Proc. Int. Conf., 3rd, 1971*, 1971, **2**, 559; *CA*, 1973, **78**, 131564 (*dodecahydrate, thermal anal*)
Pannetier, G. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 485 (*analogues*)
Strupler, N. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 1830 (*dodecahydrate, ir*)
Eysel, H.H. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **424**, 68 (*raman*)
Hurlburt, H.Z., *Encycl. Chem. Process. Des.*, 1977, **3**; *CA*, 1978, **88**, 193727 (*rec*)
Couchot, P. *et al*, *Rev. Chim. Minér.*, 1978, **15**, 373 (*anhydrous, ir, raman*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 250.
Bhat, S.V. *et al*, *Curr. Sci.*, 1984, **53**, 27 (*Al-27 nmr, anhydrous*)
Eckert, H. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2140 (*dodecahydrate, S-33 nmr*)

$AlKO_8Si_3$ IC-000204

Orthoclase

[12251-44-4]

$K[AlSi_3O_8]$

M 278.3
Open feldspar struct. with framework of $(Al,Si)O_4$ tetrahedra and 9-coord. K in interstices. At 1.2×10^5 atm. and 900° transforms to hollandite struct. with both Al and Si 6-coord. Widely distributed mineral; synthetic form obt. from oxide melts. White cryst. Sanidine and Microline are related minerals.

Cole, W.F. *et al*, *Acta Crystallogr.*, 1949, **2**, 280 (*cryst struct*)
Jones, J.B. *et al*, *Acta Crystallogr.*, 1961, **14**, 443 (*cryst struct*)
Ringwood, A.E. *et al*, *Acta Crystallogr.*, 1967, **23**, 1093 (*high press form, phase trans, props*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 4889 (*Si-29 nmr*)

$AlKSe_2$ IC-000205

Aluminium potassium selenide ($AlKSe_2$)

Potassium diselenidoaluminate. Potassium diselenoxoaluminate(1–), 9CI

$K[AlSe_2]$

M 224.0
Struct. resembles $KGaTe_2$. Synth. from elements at 980°. Yellow translucent moisture-sensitive plates (melt).

Weis, J. *et al*, *Z. Naturforsch., B*, 1976, **31**, 1336 (*synth, props*)

$AlKTe_2$ IC-000206

Aluminium potassium telluride ($AlKTe_2$)

Potassium ditelluroxoaluminate(1–). Potassium ditelluridoaluminate

[61231-60-5]

$K[AlTe_2]$

M 321.2
Struct. resembles $Tl(I)Tl(III)Se_2$ struct. Synth. from elements at 980°. Brittle red moisture-sensitive plates (melt).

Weis, J. *et al*, *Z. Naturforsch., B*, 1976, **31**, 1336 (*synth, props*)

$AlLiO_2$ IC-000207

Aluminium lithium oxide ($AlLiO_2$)

[12003-67-7]

$LiAlO_2$

M 65.9
Commercially available. Related hydrates descr. Al may be replaced by Fe. $LiAl_5O_8$ also descr.

α-form
Low pressure-form
Tetragonal with 4-coordinate Al. Synth. from Li_2CO_3 + $Al(OH)_3$ or γ-Al_2O_3 at 600-700°. Deliquescent white solid. Forms mixed cryst. with spinel and β-quartz. ΔH_f° –1189.5 kJ mol^{-1}; S° 53.3 JK^{-1} mol^{-1} *cf.* Lithium aluminate ($Li_5(AlO_4)$), IC-000212.

β-form
Mid pressure-form
Monoclinic with 4- and 6-coordinate Al. Synth. from LiOH + Al_2O_3 at 1.8×10^4 atm. and 370° or from γ-Al_2O_3, Li_2CO_3 and K_2CO_3 at 450°.

γ-form
High pressure form
Hexagonal with 6-coordinate Al; isostructural with $NaHF_2$. From Li_2CO_3 + Al_2O_3 at 3×10^4 atm. and 850°. White solid.

Bertaut, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1956, **243**, 1219 (*struct*)
Lehman, H.-A. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **313**, 117 (*synth, γ-form*)
Marezio, M., *Acta Crystallogr.*, 1966, **19**, 396 (*cryst struct, α-form*)
Marezio, M. *et al*, *J. Chem. Phys.*, 1966, **44**, 3143 (*synth, γ-form*)
Beal, G.H. *et al*, *J. Am. Ceram. Soc.*, 1967, **50**, 181 (*phase diagram*)
Tarte, P. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2127; 1970, **26**, 747 (*ir*)
Chang, C.H. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 2020 (*synth, β-form*)
Lileev, I.S. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 213 (*hydrates*)
Moore, R.K. *et al*, *J. Am. Ceram. Soc.*, 1970, **53**, 679 (*ir*)
Doman, R.C. *et al*, *J. Mater. Sci.*, 1973, **8**, 189 (*system with MgO*)
Kolesova, V.A., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 1585 (*ir*)
Fischer, A.K., *Inorg. Chem.*, 1977, **16**, 974 (*synth, β-form*)
Kinoshita, K. *et al*, *Mater. Res. Bull.*, 1978, **13**, 445 (*synth, props*)
Follstaedt, D.M. *et al*, *Phys. Rev. B: Condens. Matter*, 1978, **18**, 5928 (*Li-7 nmr*)
Müller, D. *et al*, *Polyhedron*, 1983, **2**, 1195 (*Al-27 nmr*)

$AlLiO_4Si$ IC-000208

Zeolite Li-A

$Li[AlSiO_4].H_2O$

M 126.0
Zeolite struct. ABW with 1D channels (340 × 380 pm across). Member of Phillipsite group. Synth. from silica gel, $Al_2O_3.3H_2O$ and LiOH at 250° for 36-60 hrs. or from metakaolin, silica and LiOH at 80-160°. Absorbs NH_3 but not N_2, propane. Rod like white cryst. Gallosilicate ABW also descr.

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1951, 1267 (*synth*)
Denk, G. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **382**, 209 (*synth*)
Kerr, I.S. *et al*, *Z. Kristallogr.*, 1974, **139**, 186 (*cryst struct*)
Klinowski, J. *et al*, *J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Newsam, J.M., *J. Chem. Soc., Chem. Commun.*, 1986, 1295 (*synth, cryst struct, gallosilicate*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 12.

$AlLiO_4Si$ IC-000209

Spodumene

Triphane. Lithium aluminosilicate ($LiAlSi_2O_6$). Aluminium lithium silicate ($AlLiSi_2O_6$)

[1302-37-0]

$LiAl[Si_2O_6]$

M 186.0
A pyroxene. Mineral occurs in granite pegmatites. White cryst. (aq. melt), Mp 1430°. Several modifications and related lithium aluminosilicates descr.

Monoclinic-form
Mineral (Branchville USA). Mined for its Li content. Metasilicate struct. with Al and Li octahedrally coord. Varieties include Hiddenite (green) and Kunzite (pink) which are gemstones.

Tetragonal-form
Obt. by heating $Li_2O.Al_2O_3.4SiO_2$ glass. Related to Keatite (SiO_2) with Al replacing Si and Li in interstices.

Hexagonal-form
Obt. by heating $Li_2O.Al_2O_3.4SiO_2$ glass. Related to high quartz with Al replacing Si and Li in interstices.

[12068-40-5]

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1951, 1267 (*synth, powder struct*)
Beal, G.H. *et al*, *J. Am. Ceram. Soc.*, 1967, **50**, 181 (*phase diagram*)
Li, C.-T., *Z. Kristallogr.*, 1967, **126**, 46; 1968, **127**, 327; 1973, **132**, 118 (*cryst struct*)
Clarke, P.T. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1969, **130**, 420 (*cryst struct*)
Li, C.-T., *Acta Crystallogr., Sect. B*, 1971, **27**, 1132 (*cryst struct*)
Cameron, M. *et al*, *Am. Mineral.*, 1973, **58**, 594 (*cryst struct*)
Graham, J., *Am. Mineral.*, 1975, **60**, 919 (*cryst struct*)
Harley, S.F. *et al*, *J. Chem. Phys.*, 1976, **64**, 4815 (*Al-27 nmr*)
Smith, K.A. *et al*, *Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)
Magi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)
Janes, N. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 6769 (*Si-29 nmr*)

$AlLiO_{10}Si_4$ IC-000210

Petalite

[1302-66-5]

$LiAl[Si_2O_5]_2$

M 306.2
Regarded as either a layer silicate $LiAl[Si_2O_5]_2$ or a framework silicate $Li[AlSi_4O_{10}]$. Mineral. Monoclinic; white, grey, sometimes pink or green cryst.

▷ OJ5580000.

Effenberger, H., *Tschermaks. Miner. Petrogr. Mitt.*, 1980, **27**, 129 (*cryst struct, ir*)
Tagai, T. *et al*, *Z. Kristallogr.*, 1982, **160**, 159 (*cryst struct*)
Cerny, P. *et al*, *Tschermaks. Miner. Petrogr. Mitt.*, 1983, **31**, 81 (*cryst struct*)
Magi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

$AlLi_3N_2$ IC-000211

Aluminium lithium nitride ($AlLi_3N_2$)

Li_3AlN_2

M 33.9
Has a fluorite superstruct. Synth. from Li_3N and Al at 730°. White to grey moisture-sensitive solid. Stable below 1000°.

Juza, R. *et al*, *Z. Anorg. Allg. Chem.*, 1948, **257**, 13 (*synth, props*)

$AlLi_5O_4$ IC-000212

Lithium aluminate ($Li_5(AlO_4)$)

Aluminium lithium oxide ($AlLi_5O_4$)

[12355-58-7]

$Li_5[AlO_4]$

M 125.6
Orthorhombic α-form transforms to orthorhombic β-form at 700-750°; struct. of β-form is related to Li_2O. Synth. from Li_2O and Al_2O_3. Ionic conductor: possible applications in batteries. Blanket material in nuclear power industry. Colourless cryst. (melt). Al may be replaced by Fe(*III*).

Lehmann, H.-A. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **315**, 14 (*synth, powder struct*)
Malve, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1971, **273**, 888 (*related compds*)
Stewner, F. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **380**, 241; **381**, 149; **430**, 211 (*cryst struct*)
Raistrick, I.D. *et al*, *Mater. Res. Bull.*, 1976, **11**, 953 (*electrical props*)
Follstaedt, D.M. *et al*, *Phys. Rev. B: Condens. Matter*, 1978, **18**, 5928 (*Li-7 nmr*)

[AlMg] IC-000213

Aluminium-magnesium system

Aluminium magnesium (***Al_3Mg_2***) [12004-68-1]
Al_3Mg_2 M 129.5
The β-phase in the Mg-Al system. Metallic cryst.

Riederer, K., *Z. Metallk.*, 1936, **28**, 312 (*formn*)
Samson, S., *Acta Crystallogr.*, 1965, **19**, 401 (*cryst struct*)

[AlMo] IC-000214

Molybdenum-aluminium system

Aluminium molybdenum

Alloy. Several phases known including $Mo_{20}Al$, MoAl, $MoAl_7$. Liquid Al is v. reactive towards Mo owing to its solubility in the liquid phase.

Molybdenun aluminium (***$MoAl_3$***) [12043-36-6]
Transforms to $MoAl_5$.

Molybdenum aluminium (***$MoAl_4$***) [12380-24-4]
Al_4Mo M 203.8
Obt. from Mo and Al in the liquid state. Iron-grey to black cryst.

Molybdenum aluminium (***$MoAl_5$***) [12253-69-9]
Al_5Mo M 230.8
Hexagonal struct., isotypic with Al_5W. Obt. by reaction of liq. Mo and Al. Of interest as cathode for an electrolytic cell for Al production from melt.

Molybdenum aluminium (***$MoAl_{12}$***) [12043-94-6]
$Al_{12}Mo$ M 419.7
Bcc struct., isotypic with $Al_{12}W$. Obt. by reaction of Mo and Al, in the liq. state.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1931, **11**, 523.
Malinovskii, R.R. *et al*, *CA*, 1969, **74**, 116809c (*cryst growth, $MoAl_5$*)
Vengrenovich, R.D. *et al*, *Izv. Akad. Nauk SSSR, Met.*, 1970, 186 (*struct, $MoAl_3$, $MoAl_5$*)
Pascal, P., *Compléments au Nouveau Traité de Chimie Minérale*, Masson, 1976, **5**, 2.

AlN IC-000215

Aluminium nitride (AlN)

[24304-00-5]

AlN

M 40.9
Wurtzite struct. Synth. from Al and N_2 or Al_2O_3, C and N_2 at 1400-1900°; from R_nAlNH_3 or Cl_nAlNH_{3-n} at 1200°; info. by chemical vapour deposition methods. Used in high power integrated circuits and acoustic devices. Refractory. Hard. Commercially available. White or pale greenish needles. Stable to acid. Slow dec. in hot conc. alkali. Mp >2400°. E_g 6.2 eV. Electrical cond. $10^{-6}\ \Omega^{-1}\ m^{-1}$. Thermal cond. 320 W m^{-1} K^{-1}. Relative permittivity 4.8. ΔH_f° 298 −318 kJ mol^{-1}. S_{298}° 20.1 J K^{-1} mol^{-1}.

Jaffe, G.A. *et al*, *J. Chem. Phys.*, 1976, **25**, 1024 (*cryst struct*)
Rustan, T., *Z. Anorg. Allg. Chem.*, 1976, **298**, 22 (*synth, props*)
Taylor, K.M. *et al*, *J. Electrochem. Soc.*, 1980, **107**, 809 (*synth, powder*)
Compound Semiconductors, Willardson, R.K. *et al*, Reinhold, 1962 (*synth*)
Van Vechten, J.A., *Phys. Rev.*, 1969, **182**, 891 (*props*)
McAdam, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pr*)
O'Keefe, M. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3519 (*cryst struct*)
Kuramoto, N. *et al*, *J. Mater. Sci. Lett.*, 1984, **3**, 471 (*props, use*)
Pierr, D., *Ceram. Eng. Sci. Proc.*, 1985, 1303 (*use*)
Kurokawa, Y. *et al*, *J. Am. Ceram. Soc.*, 1988, **71**, 588 (*synth, props*)
Marchant, D.D. *et al*, *Adv. Ceram.*, 1985, **26**, 19 (*use*)
Kuramoto, N. *et al*, *Ceram. Bull.*, 1989, **68**, 883 (*props, use*)
Kubota, K. *et al*, *J. Appl. Phys.*, 1989, **66**, 2984 (*props*)

IC-000216

AlN_3O_9

Aluminium nitrate

[13473-90-0]

$Al(NO_3)_3$

M 212.9
Obt. by thermal dec. of $Al(NO_3)_3.N_2O_5$. White v. hygroscopic solid. $Bp_{0.01}$ 50°. Dec. >65° to oxides.
▷ Explodes with Et_2O or C_6H_6. BD1040000.

Nonahydrate: [7784-27-2]. *Hexaaquaaluminium(3+) trinitrate trihydrate*
Synth. from HNO_3 and $Al(OH)_3$. Commercially available. Colourless plates. Sol. H_2O, Me_2CO, alcohols. Mp 73.5°. Formulated as $[Al(OH_2)_6]^{\oplus 3}[NO_3^\ominus].3H_2O$. Dec. above 130°.
▷ BD1050000.

N_2O_5 adduct:
AlN_5O_{14} M 321.0

[25549-23-9]

Archambault, J.D. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **17**, 130 (*synth*)
Addison, C.C. *et al*, *J. Chem. Soc. A*, 1966, 1434 (*synth, ir*)
Messier, D.R. *et al*, *Am. Ceram. Soc. Bull.*, 1972, **51**, 692 (*dta*)
Shirokova, G.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 799 (*synth, props*)
Krivtsov, N.V. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1741 (*thermodyn props*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 217.
Herrmann, K., *Acta Crystallogr., Sect. C*, 1983, **39**, 925 (*struct, nd*)

$AlN_4O_{12}^\ominus$

IC-000217

Tetrakis(nitrato)aluminate(1−)

Tetranitratoaluminate(1−)

$[Al(NO_3)_4]^\ominus$

M 275.0 (ion)

K salt: [59400-38-5].
$AlKN_4O_{12}$ M 314.0

From $AlBr_3$, HNO_3, KNO_3 and N_2O_5. Not obt. pure.

Rb salt: [58629-15-3].
From $RbAlCl_4$, N_2O_5 and HNO_3. Colourless hygroscopic cryst. ΔH_f° −1460.2 kJ mol^{-1}.

Cs salt: [33615-29-1].
From $CsNO_3$, $AlBr_3$, N_2O_5 and HNO_3. Colourless hygroscopic cryst. Mp 101-125° dec. ΔH_{crs}° −1469.8 kJ mol^{-1}.

Nitronium salt: [15670-61-8]. *Nitryl tetranitratoaluminate(1−)*
M 321.0
AlN_5O_{14}
From $AlBr_3$ and N_2O_5. White hygroscopic cryst. Sol. H_2O. Mp 85-98° dec. Oxidises alkanes. ΔH_f −997.0 kJ mol^{-1}.

Et_4N salt: White v. hygroscopic solid. Sol. $MeNO_2$, MeCN; spar. sol. EtOAc.
▷ Explodes on heating.

[61816-91-9]

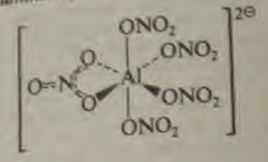
Addison, C.C. *et al*, *J. Chem. Soc. A*, 1966, 1434 (*synth, ir*)
Shirokova, G.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 1106, 1699; 1976, **21**, 527 (*synth, ir*)
Krivtsov, N.V. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 503; 1976, **21**, 1741 (*thermodyn props*)
Shirokova, G.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 856 (*synth, ir*)

IC-000218

$AlN_5O_{15}^{2\ominus}$

Pentakis(nitrato)aluminate(2−)

Pentanitratoaluminate(2−)



M 337.0 (ion)

Di-K salt: [61436-13-3].
$AlK_2N_5O_{15}$ M 415.2
Synth. from $AlBr_3$, KNO_3 and N_2O_5. Colourless moisture-sensitive cryst. ΔH_{f298}° −1966.9 kJ mol^{-1}.

Di-Rb salt: [56629-16-4].
Synth. from $AlBr_3$, $RbNO_3$, N_2O_5, and HNO_3 at −40°. Colourless v. hygroscopic cryst. (N_2O_5/HNO_3). Sol. $MeNO_2$, EtOAc; insol. CCl_4, $CHCl_3$. ΔH_f° −1982.8 kJ mol^{-1}. Dec. at 175-200°.

Di-Cs salt: [34032-04-7].
Synth. from $AlBr_3$, $CsNO_3$, N_2O_5 and HNO_3 at −40°. Colourless moisture-sensitive cryst. ΔH_f° −1999.1 kJ mol^{-1}. Dec. at 192-214°.

[59400-36-1]

Shirokova, G.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 808, 1106 (*synth*)
Dyachenko, O.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 595 (*cryst struct*)
Krivtsov, N.V. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 503; 1976, **21**, 1741 (*thermodyn props*)
Shirokova, G.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 856; 1976, **21**, 527 (*synth, ir, props*)

IC-000219

AlN_9

Aluminium(*III*) azide

[39108-14-0]

$Al(N_3)_3$

M 153.0

Synth. from AlH_3-Et_2O + HN_3 at −116° or from $AlCl_3$ + NaN_3 in C_6H_6 or THF. Used *in situ*. Reagent for synth. of tetrazoles. White moisture sensitive solid. Sol. THF; insol. Et_2O, C_6H_6.
▷ Explosive, sensitive to percussion.

Wiberg, E. *et al*, *Z. Naturforsch., B*, 1954, **9**, 495, 496, 497 (*synth, props*)
Arnold, C. *et al*, *J. Org. Chem.*, 1969, **34**, 1141 (*use*)
Wiberg, N. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **394**, 197 (*analogues*)
Wagner, E.R., *J. Org. Chem.*, 1973, **38**, 2976 (*use*)

$AlNaO_2$

IC-000220

Aluminium sodium oxide ($AlNaO_2$)

Sodium aluminium oxide ($NaAlO_2$). Sodium aluminate ($NaAlO_2$)

[1302-42-7]

$NaAlO_2$

M 81.9
$NaFeO_2$ type struct. α-form obt. from Al_2O_3 and Na_2CO_3 or from Aluminium hydroxide ($Al(OH)_3$), IC-000179 and NaOH. β-form is formed at 1.1 x 10^4 atm. at 900°. α and β designation is reversed in earlier literature. Used in water treatment, sizing of paper; raw material for manuf. of zeolites, ceramics and catalysts in petroleum industry. White cryst. or powder. Mp >1700°. Various hydrated forms known, cf. also Aluminium sodium oxide (Al_3NaO_8), IC-000373. For species in soln. see Aluminate ($Al(OH_4)^\ominus$), IC-000184. $\Delta H_{f\ 298}^\circ$ −1133.2 kJ mol^{-1}; S° 70.4 J K^{-1} mol^{-1}.

Théry, J. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1962, **254**, 2782 (*related compds*)
Reid, A.F., *Inorg. Chem.*, 1968, **7**, 443 (*cryst struct*)
Peterson, G.E. *et al*, *J. Chem. Phys.*, 1969, **51**, 2610 (*Na-23 nqr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 312.
Müller, D. *et al*, *Chem. Phys. Lett.*, 1981, **79**, 59 (*Al-27 nmr*)

$AlNaO_4Si$

IC-000221

Nepheline

[1302-72-3]

$Na[AlSiO_4]$

M 142.0
Stuffed tridymite struct. Mineral. White cryst. (aq. melt). Hydrothermal synth. from Na_2O, Al_2O_3, SiO_2 gels.

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1952, 1561 (*synth*)
Hahn, T. *et al*, *Z. Kristallogr.*, 1955, **106**, 308 (*cryst struct*)
Brinkman, D. *et al*, *Z. Kristallogr.*, 1972, **135**, 208 (*Na-23, Al-27, Si-29 nmr*)
Klaska, R. *et al*, *Z. Kristallogr.*, 1975, **142**, 225 (*cryst struct*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 4889; 1986, **108**, 1730 (*Si-29, Al-27 nmr*)
Wirsching, U., *Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Klinowski, J. *et al*, *J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)

$AlNaO_6Si_2$

IC-000222

Jadeite

Jade

[12003-54-2]

$Na[AlSi_2O_6]$

M 202.1
Common pyroxene mineral found in metamorphic rocks. An ornamental stone. Solid, various colours; on heating gives a glass from which Albite, IC-000224 and Nepheline, IC-000221 crystallise. Fe containing specimens are green or lavender. ΔH_f° −3029.9; ΔG_f° −2851.3 kJ mol^{-1}. The term Jade may refer to this mineral or to the Nephrite variety of Actinolite.

[1333-75-1]

Prewitt, C.T. *et al*, *Am. Mineral.*, 1966, **51**, 956 (*cryst struct*)
Cameron, M. *et al*, *Am. Mineral.*, 1973, **58**, 594 (*cryst struct*)
Rossman, G.R., *Am. Mineral.*, 1974, **59**, 868 (*vis*)
Hemingway, B.S. *et al*, *Am. Mineral.*, 1981, **66**, 1202 (*thermodyn*)
Mägi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

$AlNaO_8S_2$

IC-000223

Aluminium sodium sulfate ($AlNa(SO_4)_2$)

Sulfuric acid, aluminium sodium salt (2:1:1), 8Cl

[10102-71-3]

$NaAl(SO_4)_2$

M 242.0
Synth. by pptn. from aq. solns. of Na and Al sulphates with conc. sulfuric acid. Orthorhombic cryst. V. sol. H_2O (40.9 g per 100 cm^3 at 20°).

Dodecahydrate: [7784-28-3]. *Sodium alum. γ-Alum. Hexaaquaaluminium hexaaquasodium sulfate (1:1:2). Sodium aluminium sulfate ($NaAl(SO_4)_2$)*
$AlH_{24}NaO_{20}S_2$ M 458.2
Obt. by evap. or pptn. from aq. solns. containing Na and Al sulfates. Occurs as Mendozite. Food additive (baking powder); flame retardant. Cubic white cryst. Mp 61°. ΔH_f° −2353 kJ mol^{-1}. Formulated as $[Na(OH_2)_6][Al(OH_2)_6](SO_4)_2$.

Steele, F.A., *Science (Washington, D.C.)*, 1928, **68**, 156 (*dodecahydrate, synth*)
Lipson, H., *Proc. R. Soc. London, A*, 1935, **151**, 347 (*dodecahydrate, cryst struct*)
Cola, M., *Gazz. Chim. Ital.*, 1960, **90**, 220 (*cryst struct, synth*)
Cromer, D.T. *et al*, *Acta Crystallogr.*, 1967, **22**, 182 (*dodecahydrate, cryst struct, nd*)
Petrov, K.I. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 2938 (*dodecahydrate, ir*)
Perret, R. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 366 (*synth*)
Weiden, N. *et al*, *J. Magn. Reson.*, 1975, **20**, 279 (*dodecahydrate, Na-23, Al-27 nmr*)
Hurlburt, H.Z., *Encycl. Chem. Process. Des.*, 1977, **3**, 120; *CA*, 1978, **88**, 193727 (*rev, synth*)
WHO Tech. Rep. Ser., 1978, **631**, 7; *CA*, 1979, **90**, 136443 (*uses*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 244 (*dodecahydrate, rev*)

$AlNaO_8Si_3$

IC-000224

Albite

Sodium aluminosilicate ($NaAlSi_3O_8$)

[12244-10-9]

$Na[AlSi_3O_8]$

M 262.2
Feldspar struct. with 3-D 4-connected net of AlO_4 and SiO_4 tetrahedra. Na 7 or 8 coord. Several modifications. May contain up to 10 Mol.% $CaAl_2Si_2O_8$, see Anorthite, IC-000262. Mineral, occur. widespread. White cryst. (aq. melt).

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1952, 1561 (*synth*)
Ferguson, R.B. *et al*, *Acta Crystallogr.*, 1958, **11**, 331 (*cryst struct*)
Ribbe, P.H. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 1503 (*cryst struct*)
Prewitt, C.T. *et al*, *Am. Mineral.*, 1976, **61**, 1213 (*cryst struct*)
Winter, J.K. *et al*, *Am. Mineral.*, 1977, **62**, 921 (*props*)
Harlow, G.E. *et al*, *Am. Mineral.*, 1980, **65**, 986 (*cryst struct, nd*)

Lippmaa, E. *et al, J. Am. Chem. Soc.*, 1980, **102**, 4889; 1986, **108**, 1730 (*Si-29 nmr*)
Smith, K.A. *et al, Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)

IC-000225

$AlNaSe_2$

Aluminium sodium selenide ($AlNaSe_2$)

Sodium diselenoxoaluminate(1–), 9CI. Sodium diselenidoaluminate

[61216-36-2]

$Na[AlSe_2]$

M 207.8

Struct. resembles Tl(*I*)Tl(*III*)Se_2. Synth. from elements at 980°. Pale yellow soft, air- and moisture-sensitive cryst. (melt).

Weis, J. *et al, Z. Naturforsch., B*, 1976, **31**, 1336 (*synth, props, cryst struct*)

IC-000226

$AlNaTe_2$

Aluminium sodium telluride ($AlNaTe_2$)

Sodium ditelluroxoaluminate(1–), 9CI. Sodium ditelluridoaluminate

[61216-37-3]

$Na[AlTe_2]$

M 305.1

Struct. resembles Tl(*I*)Tl(*III*)Se_2. Synth. from elements at 980°. Soft red, air- and moisture-sensitive plates (melt).

Weis, J. *et al, Z. Naturforsch., B*, 1976, **31**, 1336 (*synth, props, cryst struct*)

IC-000227

$AlNa_5O_4$

Sodium aluminate ($Na_5(AlO_4)$)

Pentasodium aluminate ($AlO_4^{5\ominus}$). Aluminium sodium oxide ($AlNa_5O_4$)

[54723-33-0]

$Na_5[AlO_4]$

M 205.9

Struct. contains isolated $[AlO_4]^{5\ominus}$ tetrahedra. Obt. from solid state reaction between Na_2O and Al_2O_3 at 700°. V. hygroscopic white solid.

Barker, M.G. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 379 (*synth, cryst struct*)

IC-000228

$AlNbO_4$

Aluminium(*III*) niobium(*V*) oxide ($AlNbO_4$)

Aluminium niobate

[12258-25-2]

$AlNbO_4$

M 183.8

AlO_6 and NbO_6 octahedra share edges and corners. Synth. from Nb_2O_5 + Al_2O_3. Colourless plates (melt).

Pedersen, B.F., *Acta Chem. Scand.*, 1962, **16**, 421 (*synth, cryst struct*)

$AlO_2^{\ominus}$

Aluminate ($AlO_2^{\ominus}$) **IC-000229**

[20653-98-9]

$[AlO_2]^{\ominus}$

M 58.9 (ion)

May be species in dehydration of $Al(OH)_4^{\ominus}$ in presence of $Na^{\oplus}$. Detected by ms. ΔH_f^o (g) −582.8 kJ mol^{-1}.

Li salt: see *Aluminium lithium oxide ($AlLiO_2$)*, IC-000207

Na salt: see *Aluminium sodium oxide ($AlNaO_2$)*, IC-000220

K salt: see *Aluminium potassium oxide ($AlKO_2$)*, IC-000201

Mg salt: see *Aluminium magnesium oxide (Al_2MgO_4)*, IC-000309

Ca salt: see *Aluminium calcium oxide (Al_2CaO_4)*, IC-000261

Sr salt: see *Aluminium strontium oxide (Al_2SrO_4)*, IC-000323

Ba salt: see *Aluminium barium oxide (Al_2BaO_4)*, IC-000245

Carreira, L.A. *et al, J. Chem. Phys.*, 1966, **45**, 2216 (*ir, raman*)
Srivastava, R.D. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 1388 (*ms*)
Müller, D. *et al, Chem. Phys. Lett.*, 1981, **79**, 59 (*Al-27 nmr*)

IC-000230

[AlO_2PSi]

Silicoaluminophosphate molecular sieves

SAPO

$(Si_xAl_yP_z)O_2$, x = 0.01-0.98, y = 0.01-0.6, z = 0.01-0.52; $x + y + z = 1$

A class of crystalline microporous framework oxides exhibiting at least 13 3D structures most of which are topologically related to the zeolites and aluminophosphates. Synth. hydrothermally from an org. amine + $Al_2O_3.nH_2O$ + phosphoric acid + silica sol. Cryst. Props. are related to both the zeolites and aluminophosphates.

Wilson, S.T. *et al, J. Am. Chem. Soc.*, 1982, **104**, 1146.
Artioli, G. *et al, Acta Crystallogr., Sect. C*, 1984, **40**, 214 (*cryst struct*)
Lok, B.M. *et al, J. Am. Chem. Soc.*, 1984, **106**, 6092 (*synth, props*)
Ito, M. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 1698 (*cryst struct*)

AlO_4P **IC-000231**

Aluminium phosphate (1:1), 9CI, 8CI

Aluminium orthophosphate

[7784-30-7]

$AlPO_4$

M 121.9

Exists in various mineral and polymorphic forms. Forms acid salts with H_3PO_4, and intercalation compds. with e.g. organic bases. Forms basis of numerous microporous compositions with zeolitic character. A wide range of other elements may be incorporated. Employed as refractory material e.g. in binders and in bricks. With other metal oxides forms highly coloured materials useful as pigments. Employed in some dental and pharmaceutical prepns. Commercially available.

▷ TB6450000.

Sesquihydrate: [99835-04-8].
Sq. prismatic needles. Orthorhombic lattice with linked AlO_4 and PO_4 tetrahedra and $AlO_4(H_2O)_2$ octahedra and encapsulated H_2O.

Dihydrate: [13477-75-3].
Synth. from NaH_2PO_4, $AlCl_3$, NaOH aq., pH 3.8 at 60-90° → Variscite. $Al_2(SO_4)_3$ + Na_3PO_4 aq. at <135° → Metavariscite. Normally minute hexagonal plates.

Trihydrate: [22784-12-9].
Colourless, elongated hexagonal plates. Dehydrates at <400°, → cristobalite form.

Compd. with [NMe_4]OH: [104422-12-0]. *$AlPO_4$ - 12TMAU*
$C_4H_{13}Al_3NO_{13}P_3$ M 457.0

Obtained hydrothermally at 200°. White cryst.

Compd. with ethylenediamine (3:1) and 1H_2O: [96360-79-1].
$AlPO_4$21(en)
$C_2H_{10}Al_3N_2O_{13}P_3$ M 443.9
Obt. hydrothermally at 200°. White cryst. + 1H_2O.
Formulated as $Al_3(PO_4)_3(H_2NCH_2CH_2NH_2).H_2O$.

Compd. with pyrrolidine (3:1) and 1H_2O: [96360-80-4].
$AlPO_4$21(pyrrolidine)
$C_4H_{11}Al_3NO_{13}P_3$ M 454.9
Obt. hydrothermally at 150°. White prisms.

Compd. with piperidine hydrate: $AlPO_4$-17
Obt. from gel at 200°. Related to Erionite. Formulated as $Al_{18}(PO_4)_{18}.4(C_5H_{11}N.H_2O)$.

Clathrate with 1H_2O and 1 ethylenediamine: [98218-54-3].
$AlPO_4$-12(en)
$C_2H_{10}Al_3N_2O_{13}P_3$ M 443.9
Colourless cryst. (aq. melt).

Amorph.-form
Composition approximates to that of the trihydrate. Cryst. as berlinite at 525°.

Quartz-form
From Al_2O_3 + H_3PO_4; from Aluminium phosphate ($Al(H_2PO_4)_3$), IC-000188 at 1100-1300°, by dehydration of metavariscite at 240-800°; or from $NaAlO_2$ + H_3PO_4. Also obt. as mineral. Transparent prisms. The low-temp. α-form is transformed into the high-temp. β-form at 580-585°; the latter at >650° yields the high temp. tridymite form.

Tridymite-form
Hexagonal lattice. By dehydration of variscite at 900°; from $Al(NO_3)_3$ + Ammonium phosphate ($(NH_4)(H_2PO_4)$), IC-019726. The low-temp. and high-temp. forms interconvert 90°; the high temp. form being obt. from β-quartz form at 650°, and at >1000° yields the high temp. cristobalite form.

Cristobalite-form
Orthorhombic or cubic lattice with transformation at *ca* 100°. From the trihydrate at <400°. The high temp. tridymite form at >1000°→ high temp. cristobalite form (dec. at >1330°), which on cooling (189°) affords the low temp. cristobalite form. The transformation low→ high temp. cristobalite occurs at 208°. Mp >1600°.

Mineral-form [13769-32-9]
Berlinite
Essentially the anhydrous salt. With the α-quartz struct. Greyish to pale white, transparent to translucent, cryst. resembling quartz. Crysts. easily twin. Undergoes phase transition at 584°.

Mineral-form [14752-50-2]
Metavariscite
Essentially the dihydrate. Monoclinic cell in which the PO_4 tetrahedra share vertices with four $AlO_4(OH_2)_2$ octahedra, and vice-versa. The H_2O molecules are coordinated *cis*. P-O 152.8-154.2 pm, OPO 107.1-112.1°. Found in Tadzhikistan and the USA (Arkansas, Utah).

Mineral-form [13824-50-5]
Variscite
Essentially the dihydrate. Orthorhombic. Found in S. and W. Australia, Europe (Germany, Austria, Czechoslavakia), S. America (Venezuela, Columbia, Brazil) and southern regions of the USSR. Dipyramidal, colourless to pale green cryst. Dehydrates at 165° in single stage. When roasted at 900° consists mainly of the tridymite form with small amounts of berlinite.

Mineral-form
Richmondite
Essentially the tetrahydrate.

Dana's System of Mineralogy, 7th Ed., **II**, 696, 756, 762.

Jameson, R.F. *et al, J. Chem. Soc.*, 1954, 4013 (*synth*)
d'Yvoire, F., *Bull. Soc. Chim. Fr.*, 1961, 1762 (*synth, powder struct*)
Brun, E. *et al, Helv. Phys. Acta*, 1961, **34**, 388 (*electric field grad tensor*)
Arlidge, E.Z. *et al, J. Appl. Chem.*, 1963, **13**, 17 (*synth, ir*)
Tarte, P., *Bull. Soc. Chim. Fr.*, 1968, 1750 (*ir*)
Christynkova, A.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 536; *Inorg. Materials (Engl. Transl.)*, 1969, **5**, 449 (*synth*)
Kobtsev, B.M. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 396; *Inorg. Materials (Engl. Transl.)*, 1972, **8**, 348 (*props*)
Kniep, R. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 2292; 1977, **33**, 263 (*cryst structs, metavariscite and variscite*)
Dorémieux-Morin, C. *et al, Bull. Soc. Chim. Fr.*, 1973, 409 (*synth, pmr*)
Morris, J.H. *et al, Chem. Soc. Rev.*, 1977, **6**, 173 (*use*)
Wignall, G.D. *et al, J. Mater. Sci.*, 1977, **12**, 1039 (*synth, struct*)
Allaf, K. *et al, High Temp. High Pressures*, 1978, **10**, 591 (*props*)
Greben'ko, N.V. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 136; *Inorg. Materials (Engl. Transl.)*, 1978, **14**, 105 (*synth*)
Nicola, J.H. *et al, Phys. Rev. B*, 1978, **18**, 1972 (*raman*)
Thong, N. *et al, Acta Crystallogr., Sect. A*, 1979, **35**, 658 (*cryst struct, low quartz form*)
Kosten, K. *et al, Z. Kristallogr.*, 1980, **152**, 119 (*cryst structs*)
Wilson, S.T. *et al, J. Am. Chem. Soc.*, 1982, **104**, 1146 (*rev*)
Parise, J.B. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 515 (*synth, cryst struct AlPO$_4$-21en*)
Parise, J.B. *et al, Inorg. Chem.*, 1985, **24**, 4312 (*cryst struct, AlPO$_4$-12en*)
Dietzel, A., *J. Non-Cryst. Solids*, 1985, **73**, 47 (*props*)
Müller, D. *et al, Zeolites*, 1985, **5**, 531 (*Al-27, P-31 nmr*)
Pluth, J.J. *et al, Acta Crystallogr., Sect. C*, 1986, **42**, 1118 (*synth, cryst struct, hydrates*)
Byrappa, K. *et al, J. Crystal Growth*, 1986, **79**, 232 (*synth, ir, props, morphol*)
Rudolph, P.R. *et al, J. Phys. Chem.*, 1986, **90**, 6122 (*synth, cryst struct, compd with Me$_4$NOH*)
Mudrakovskii, I.L. *et al, J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Shternberg, A.A. *et al, Kristallografiya*, 1986, **31**, 1206; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1986, **31**, 712 (*struct*)
Flanigen, E.M. *et al, Pure Appl. Chem.*, 1986, **58**, 1351 (*compds with other metals*)
Bennett, J.M. *et al, Zeolites*, 1986, **6**, 349; 1987, **7**, 160 (*rev, nd*)
Jumas, J.C. *et al, J. Crystal Growth*, 1987, **80**, 133 (*synth, phys, electrical props*)
Lowe, B.M. *et al, J. Chem. Soc., Chem. Commun.*, 1988, 1186 (*use*)
Meinhold, R.H. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 219 (*use*)
Quisheng, H. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 783 (*synth*)

AlO_4Re **IC-000232**

Aluminium rhenium(*V*) oxide ($AlReO_4$), 9CI

[53906-75-5]

$AlReO_4$

M 277.1

Rutile struct. with statistical distribution of cations. Synth. from Al_2O_3, ReO_3 and Al at 1200-1300° and 5.8 x 10^4 atm. Black powder, stable under ambient conditions. Ga and Fe(*III*) salts are similar.

Sleight, A.W., *Inorg. Chem.*, 1975, **14**, 597 (*synth, struct, props*)

$AlO_6Ti_2^{\ominus}$ **IC-000233**

Hexaoxoaluminatedititanate(*IV*)(1–), 11CI

$[AlTi_2O_6]^{\ominus}$

M 218.7 (ion)

Ba salt (2:1): [12650-43-0]. *Aluminium barium titanium*(IV) *oxide ($Al_2BaTi_4O_{12}$), 9CI*
$Al_2BaO_{12}Ti_4$ M 574.8

Synth. by heating $BaCO_3$, TiO_2 and Al_2O_3 to 1200° in a Pt container. Ceramic. Mp 1470°. Hollandite type struct.

Guha, J.P. *et al*, *J. Am. Ceram. Soc.*, 1972, **55**, 55 (*synth, thermal anal*)
U.S.S.R. Pat., 986 902, (1983); *CA*, **98**, 203307b (*use*)
Kesson, S.E. *et al*, *Proc. R. Soc. London, A*, 1986, **405**, 73 (*synth, cryst struct*)

IC-000234

AlO_9P_3

Aluminium trimetaphosphate

Metaphosphoric acid, aluminium salt. Aluminium metaphosphate

[13776-88-0]

$Al(PO_3)_3$

M 263.8

Constit. of glasses, coatings, binders and ceramics. Catalyst for esterifications and oxidation of alkenes. Several forms descr.

Monoclinic form: Obt. from Al_2O_3 and HPO_3 (melt). Struct. comprises chains of PO_4 tetrahedra connected by AlO_6 octahedra.

D'Yvoire, F., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1960, **251**, 2182 (*polymorphs*)
van der Meer, H., *Acta Crystallogr., Sect. B*, 1976, **32**, 2423 (*cryst struct*)
Morris, J.H. *et al*, *Chem. Soc. Rev.*, 1977, **6**, 173 (*rev*)

IC-000235

$AlO_{40}W_{12}^{5\ominus}$

Tungstoaluminate ($AlW_{12}O_{40}^{5\ominus}$)

Aluminatetetracosa-μ-oxotetra-μ$_4$-oxododecaoxododecatungstate(5−), 10Cl. Tetracontaoxoaluminatedodecatungstate(5−)

[68943-71-5]

$[AlW_{12}O_{40}]^{5\ominus}$

M 2873.1 (ion)

A Keggin-type heteropolyanion. Formed from $Al^{3\oplus}$ + $[WO_4]^{2\ominus}$ in acid solns.

Penta-Cs salt: [61178-77-6]. Colourless opaque prisms. Spar. sol. H_2O.

Penta-H compd.: [121328-06-1]. *12-Tungstoaluminic acid* $AlH_5O_{40}W_{12}$ M 2878.1

Prepd. in the solid state (as a hexahydrate) from its aq. soln. by the cryogenic method. Colourless solid. V. sol. H_2O.

Penta-NH$_4$ salt: Transparent, colourless octahedra. V. sol. H_2O.

[68943-71-5, 79747-17-4, 87331-89-3, 94698-85-8]

Mair, J.A. *et al*, *J. Chem. Soc.*, 1950, 2372 (*synth*)
Brown, D.H., *J. Chem. Soc.*, 1962, 3281 (*struct*)
Akitt, J.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1615 (*Al-27 nmr*)
Nomiya, K. *et al*, *Polyhedron*, 1983, **2**, 955 (*synth, ir, uv, mcd*)
Lunk, H.-J. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **568**, 171 (*synth, acid, Al-27 nmr*)

AlP

Aluminium phosphide (AlP) **IC-000236**

[20859-73-8]

AlP

M 57.9

Zinc blende struct. Synth. from Zn_3P_2 and Al at 800°. Synth. from elements in exothermic reaction. Fumigant and pesticide. Solid solns. with GaP are used in luminescence and optical devices. Grey to dark yellow moisture sensitive cryst. stable up to 1000°.

▷ Reacts with H_2O to give PH_3 (inflammable, toxic). BD1400000.

White, W.E. *et al*, *J. Am. Chem. Soc.*, 1944, **66**, 1666 (*synth*)
Inorg. Synth., 1953, **4**, 23 (*synth*)
Addamiano, A., *J. Am. Chem. Soc.*, 1960, **82**, 1537; *Acta Crystallogr.*, 1960, **13**, 505 (*cryst struct*)
Wang, C.C. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **25**, 326 (*synth, props*)
Van Vechten, J.A. *et al*, *Phys. Rev.*, 1969, **182**, 891 (*cryst struct*)
O'Keefe, M. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3519 (*cryst struct*)

$AlPS_4$

IC-000237

Aluminium tetrathiophosphate

Aluminium phosphorotetrathioate. Aluminium thiophosphate

[98987-28-1]

$AlPS_4$

M 186.2

Struct. comprises edge-sharing tetrahedral chains similar to SiS_2. Prepd. by heating AlP in a S atm. at 650°. Colourless needles and plates. V. hygroscopic. Dec. in air with evolution of H_2S.

Weiss, A. *et al*, *Naturwissenschaften*, 1960, **47**, 495 (*cryst struct*)
Wibbelmann, C. *et al*, *Z. Naturforsch., A*, 1985, **40**, 909 (*ir, raman*)

AlSb

IC-000238

Aluminium antimonide (AlSb)

[25152-52-7]

AlSb

M 148.7

Has zinc blende struct. Synth. from elements. Commercially available. Black solid. Mp 1080°. ΔH_f° −104.7 kJ mol^{-1}; S° 63 J K^{-1}mol^{-1}; band gap 1.62 eV; n_D 3.18. ε 10.2.

Hilsum, C. *et al*, *Semiconducting III-V Compounds*, Pergamon, Oxford, 1961.
Willardson, R.K. *et al*, *Compound Semiconductors*, Reinhold, 1962 (*synth*)
Piespergen, U. *et al*, *Z. Naturforsch., A*, 1963, **18**, 141 (*thermodyn*)
Willardson, R.K. *et al*, *Semiconductors and Semimetals*, Academic Press, 1966, **1**, 2; 1967, **3**; 1968, **4**.
Mooradian, A. *et al*, *Solid State Commun.*, 1966, **4**, 431 (*raman*)
Van Vechten, J.A. *et al*, *Phys. Rev.*, 1969, **182**, 891 (*cryst struct*)
O'Keefe, M. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3519 (*cryst struct*)

[AlSr]

IC-000239

Aluminium-strontium system

Aluminium strontium (***Al$_7$Sr$_8$***) [86899-93-6]

Al_7Sr_8 M 889.8

Formerly descr. as Sr_3Al_2 and SrAl. From elements. Metallic moisture-sensitive plates (melt).

Fornasini, M.L., *Acta Crystallogr., Sect. C*, 1983, **39**, 943 (*cryst struct*)

[AlTe]

Aluminium tellurides **IC-000240**

Aluminium telluride (***Al$_2$Te$_{10}$***) [110772-85-5]

Al_2Te_{10} M 1464.8

Struct. contains [Te_4Al_4—Al_4Te_4] units with Al—Al bonds and Al_2Te_2 rings. Synth. from elements at 927°. Air- and moisture-sensitive ruby red cryst.

Aluminium telluride (***Al$_2$Te$_3$***) [12043-29-7]

Al_2Te_3 M 436.7

Wurtzite struct. with Al in two thirds of cation sites. Synth. from elements at 1000°. Source of H_2S (D_2S) as *in situ* reducing agent for aldehydes and enones. Commercially available. Dark grey solid (melt). Mp 895°. ΔH_f° −326 kJ mol^{-1}. Band gap E_g 2.2 eV. Conductance 1.85 × 10^4 Ω^{-1}m^{-1}.

Kauer, E. *et al*, *Z. Naturforsch., A*, 1958, **13**, 531 (*optical props*)
Steigmann, G.A. *et al*, *Acta Crystallogr.*, 1966, **20**, 617 (*cryst struct*)
Gromakov, S.D. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1972, **46**, 91 (*props*)
Said, H. *et al*, *J. Less-Common Met.*, 1976, **46**, 209 (*thermodyn*)
Kambe, N. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1980, **19**, 1009 (*use*)
Nesper, R. *et al*, *Z. Naturforsch., B*, 1987, **42**, 557 (*synth, cryst struct*)

[AlU]

IC-000241

Aluminium uranium system

Main alloys are UAl_2, UAl_3, UAl_4. Used as fuel elements in high neutron-flux reactors, usually as Al-rich alloys.

Aluminium compd. with uranium (***1:4***) [12005-05-9]

Al_4U M 345.9

U has 13 Al nearest neighbours at 302-330 pm. Black needles or powder. Mp 730° dec. Dec. to UAl_3 + Al on heating. Obeys Curie-Weiss law between 293-923K (μ_{eff} = 3.2μ_B). Susceptibility temp. independent to 100K.

▷ Pyrophoric as powder.

Aluminium, compd. with uranium (***1:3***) [12004-79-4]

Al_3U M 318.9

Yellow solid. Mp 1350° dec. Prob. $AuCu_3$ struct. Dec. to UAl_2 + Al on heating. Obeys Curie Weiss law 293-1073K. μ_{eff} = 3.5μ_B.

▷ Pyrophoric as powder.

Aluminium compd. with uranium (***2:1***) [12004-48-7]

Al_2U M 291.9

$MgCu_2$ struct. U surrounded by 12 Al and 4 distant U. Mp 1590° (1620°). Paramagnetic. Obeys Curie-Weisslaw >100K. μ_{eff} = 3.0μ_B.

▷ Pyrophoric as powder.

Rundle, R.E. *et al*, *Acta Crystallogr.*, 1949, **2**, 148 (*struct, UAl_3*)
Boucher, R., *J. Nucl. Mater.*, 1959, **1**, 13 (*synth*)
Chamberlain, J. *et al*, *J. Nucl. Mater.*, 1966, **19**, 121 (*synth, UAl_2*)
Grimmet, E.S. *et al*, *Chem. Eng. Prog. Symp. Ser.*, 1967, **63**, 11; *CA*, **68**, 55712 (*synth*)
U.S. Pat., 3 318 670, (1967); *CA*, **67**, 49755 (*synth*)
Jesse, A., *J. Nucl. Mater.*, 1970, **37**, 340 (*struct, UAl_4*)
Jesse, A. *et al*, *Powder Metall.*, 1971, **14**, 289 (*use, UAl_4*)
Brodsky, M.B., *Phys. Rev. B*, 1974, **9**, 1381 (*magnetism, UAl_3, UAl_4*)
Nazare, S. *et al*, *J. Nucl. Mater.*, 1975, **56**, 251 (*synth, UAl_3, UAl_4*)
Brodsky, M.B. *et al*, *Physica B+C (Amsterdam)*, 1977, **91**, 271 (*magnetism, UAl_2*)
Fournier, J.M. *et al*, *J. Phys. Colloq.*, 1979, **40**, C4, 145 (*magnetism, UAl_2*)
Ger. Pat., 3 042 424, (1980); *CA*, **97**, 135543 (*use, UAl_4*)
Wire, M.S. *et al*, *J. Magn. Magn. Mater.*, 1985, **53**, 283 (*cryst struct, UAl_2*)
Gmelin Handbook Inorg. Chem., Syst. No. 55, Suppl. Vol., 1989, **B2**, 82 (*rev*)

$Al_{1.67}H_2Mg_{0.33}Na_{0.33}O_{12}Si_4$

IC-000242

Bentonite

[1302-78-9]

$Na_{0.33}[Al_{1.67}Mg_{0.33}Si_4O_{10}(OH)_2]$

M 367.0

Rock containing Montmorillonite, IC-000371 and var. other clay minerals. Widely distributed mineral. Used in drilling muds, foundary moulding sands, fillers, ore pellitisation fire extinguishers and in removal of radioactive waste. Constituent of Fuller's earth.

▷ CT9450000.

van Olpen, H., *Clay Colloid Chemistry*, 2nd Edn., Wiley, N. Y., 1977.
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 238, 241; **6**, 193, 200 (*rev*)

$Al_2BaH_8O_{14}Si_3$

IC-000243

Edingtonite

Glottalite

$Ba_2[Al_4Si_6O_{20}].8H_2O$

M 507.6

Zeolite struct. EDI with 2D channels (280 × 380 pm across) of $(Si,Al\text{-}O)_8$ rings and 1D channel of variable diameter of $(Si,Al\text{-}O)_8$ rings. Member of natrolite group. Rare natural zeolite mineral from Scotland, Sweden, Bohemia. Hydrothermal synth. from $BaO\text{-}Al_2O_3\text{-}SiO_2$—$H_2O$ gels. Fibrous white cryst. Void fraction 0.36 cm^3 cm^{-3}.

Breck, D.W., *Zeolite Molecular Sieves*, Wiley, London, 1974.
Galli, E., *Acta Crystallogr., Sect. B*, 1976, **32**, 1623 (*cryst struct*)
Kvick, Å. *et al*, *J. Chem. Phys.*, 1983, **79**, 2356 (*nd*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 54.

$Al_2BaH_{12}O_{22}Si_6$

IC-000244

Harmotome

[12251-39-7]

$Ba_2[Al_4Si_{12}O_{32}].12H_2O$

M 723.8

Zeolite struct. PHI with 3D channel system (420 × 440; 280 × 480; 330 pm across) with $(Al,Si\text{—}O)_8$ rings. Hydrothermal synth. at 300°. Widely distributed mineral of sedimentary and hydrothermal origin. Found in USA, Canada, Finland, New Zealand, Scotland, Wales, Norway, Germany, Italy and USSR. White cryst. Void vol. 0.31 cm^3 cm^{-3}.

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1959, 1521; 1961, 983 (*synth, Ca, Ba, Na forms*)
Sadanaga, R. *et al*, *Acta Crystallogr.*, 1961, **14**, 1153 (*cryst struct*)
Rinaldi, R. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 3426 (*cryst struct*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, London, 1974.
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4992 (*Si-29 nmr*)
Gottardi, G. *et al*, *Natural Zeolites*, Springer, 1985, 134.
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 120.

Al_2BaO_4

IC-000245

Aluminium barium oxide (Al_2BaO_4)

[12004-04-5]

$BaAl_2O_4$

M 255.2

Tridymite struct. with Ba in interstices. Synth. from BaO or $BaCO_3$—Al_2O_3—B_2O_3 melt. Used as ceramic in nuclear reactors and as support for transition metal and lanthanide phosphors. Clear hexagonal rods (melt). $Mn^{2\oplus}$ doped cryst. also descr. $Al_2Ba_3O_4$ and several other related compds. descr.

Hoppe, R. *et al*, *Naturwissenschaften*, 1960, **47**, 376 (*cryst struct*)
Glasser, F.P. *et al*, *J. Am. Ceram. Soc.*, 1963, **46**, 377 (*synth, cryst struct*)
Arlett, R.H. *et al*, *Acta Crystallogr.*, 1967, **22**, 315 (*cryst struct*)
Palilla, F.C. *et al*, *J. Electrochem. Soc.*, 1968, **115**, 642 (*phosphors*)
Do-Dinh, C. *et al*, *J. Phys. (Paris)*, 1970, **31**, 401 (*nd*)
Beretka, J. *et al*, *Aust. J. Chem.*, 1973, **26**, 2527 (*synth, reactions*)
Riebling, E.-F. *et al*, *Mater. Res. Bull.*, 1975, **10**, 997 (*synth*)
Hörkner, W. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **451**, 40 (*cryst struct*)
Sander, K. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **468**, 197 (*Mn-doped cryst*)
Müller, D. *et al*, *Chem. Phys. Lett.*, 1981, **79**, 59 (*Al-27 nmr*)
Müller, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1277 (*Al-27 nmr*)

$Al_2BaO_8Si_2$ IC-000246
Celsian
Barium feldspar
[1302-50-7]

$Ba[Al_2Si_2O_8]$

M 375.4
Struct. has open framework of $(Al,Si)O_4$ tetrahedra sharing corners, with 7-coord. Ba in the interstices. Mineral occurs mainly in contact zones of manganese deposits. Hydrothermal synth. from Kaolinite and $Ba(OH)_2$ at 100-300°. Used in manuf. of ceramics and glass, as base for var. pigments. Transparent white cryst. Several forms descr. Isomorphous replacements of Si by Ge, Al by Ga, and Ba by Sr.

Newnham, R.E. *et al*, *Acta Crystallogr.*, 1960, **13**, 303 (*cryst struct*)
Barrer, R.M. *et al*, *J. Chem. Soc.*, 1964, 2296 (*synth*)
Semler, C.E. *et al*, *J. Am. Ceram. Soc.*, 1970, **53**, 595 (*phase diagram*)
Gazzoni, G. *et al*, *Z. Kristallogr.*, 1973, **137**, 24 (*cryst struct*)
Callen, M. *et al*, *Z. Kristallogr.*, 1973, **137**, 293 (*rev, synth*)
Chiari, G. *et al*, *Am. Mineral.*, 1975, **60**, 111 (*cryst struct, Sr analogue*)
Griffin, D.T. *et al*, *Am. Mineral.*, 1976, **61**, 414 (*cryst struct*)
Ovchinnikov, N.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **234**, 1097 (*synth*)
Smolenskikh, P.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1978, **238**, 85 (*cryst struct, analogues*)

$Al_2BaO_8Si_2$ IC-000247
Paracelsian
[12337-57-0]

$Ba[Al_2Si_2O_8]$

M 375.4
$(Al,Si)O_4$ tetrahedra share corners to make open framework with 7-coord. Ba in interstices. Mineral. Hydrothermal synth. from BaO, Al_2O_3, SiO_2, H_2O at 150-375°. Similar to Celsian. IC-000246. White cryst.

Smith, J.V., *Acta Crystallogr.*, 1953, **6**, 613 (*cryst struct*)
Bakakin, V.V., *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1961, **5**, 826 (*cryst struct*)
Ovchinnikov, F.D. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1977, **13**, 2068 (*synth*)

Al_2BaS_4 IC-000248
Aluminium barium sulfide (Al_2BaS_4), 9CI
Barium thioaluminate ($Ba(Al_2S_4)$)
[51403-77-1]

$BaAl_2S_4$

M 319.5
Struct. has AlS_4 tetrahedra linked by corners and 12-coord. Ba. Cryst.

Eisenmann, B. *et al*, *Mater. Res. Bull.*, 1982, **17**, 1169 (*cryst struct*)

Al_2BaSe_4 IC-000249
Aluminium barium selenide (Al_2BaSe_4)
Barium diselenoxoaluminate(1−) (1:2)
[79470-80-7]

Al_2BaSe_4

M 507.1
Tetragonal struct. has $AlSe_4$ tetrahedra sharing corners with $BaSe_8$ antiprisms, struct. resembles TlSe. Synth. from $BaAl_2$ and Se at 1000°. Rectangular, beige, translucent moisture-sensitive cryst.

Klee, W. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **479**, 125 (*cryst struct*)

Al_2BaTe_4 IC-000250
Aluminium barium telluride (Al_2BaTe_4)
Barium ditelluridoaluminate(1−) (1:2)
[39297-18-2]

$BaAl_2Te_4$

M 701.6
Structure has $AlTe_4$ tetrahedra which share corners with $BaTe_8$ antiprisms; struct. resembles TlSe. Synth. from stoichiometric amounts of the elements at 1200°. Red air- and moisture-sensitive prisms (from melt). $Ba_7Al_6Te_{16}$ also descr.

Franke, E.R. *et al*, *Z. Naturforsch., B*, 1972, **27**, 1308 (*synth, props*)

Al_2BeO_4 IC-000251
Beryllium aluminate (1:2), 10CI
Aluminium beryllium oxide, 8CI. Beryllium dialuminium oxide ($BeAl_2O_4$)
[12004-06-7]

$BeAl_2O_4$

M 126.9
One of two ($BeAl_2O_4$; $BeAl_6O_{10}$) congruently melting compounds of the BeO—Al_2O_3 system. Prepd. by sintering equimolar mixtures of BeO and Al_2O_3. White cryst. Mp 1873°, ΔH_f° −2301 kJ mol^{-1}; ΔG_f° −2179 kJ mol^{-1}; S° 66.3 J K^{-1} mol^{-1}.

▷ Highly toxic.

Mineral-form [1304-50-3]
Chrysoberyl
Gem variety is Alexandrite which is a component of tunable lasers. Orthorhombic cryst., may be yellow to greenish.

[12252-02-7]

Swanson, H.E. *et al*, *Natl. Bur. Std. Circ. (U.S.)*, 1960, **9**, 10 (*cryst struct*)
Henning, O. *et al*, *C.A.*, 1968, **68**, 82724 (*ir*)

Walling, J.C. *et al*, *IEEE J. Quantum Electron.*, 1985, **QE-21**, 1568 (*uses*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 141 (*thermochem data*)

$Al_2Be_2Ca_4H_2O_{28}Si_9$ IC-000252
Bavenite, 9CI
[1318-17-8]

$Ca_4Be_2Al_2[Si_6O_{16}][Si_3O_{10}](OH)_2$

M 935.0
Mineral. A double chain silicate. Occurs chiefly in granite pegmatites in association with beryl. White, greenish white, pinkish, pale brown, orthorhombic needles.

[12654-22-7, 61232-54-0]

Claringbull, G.F., *Mineral. Mag.*, 1940, **25**, 475 (*occur*)
Fleischer, M. *et al*, *Am. Mineral.*, 1953, **38**, 988 (*mineral*)
Cannillo, E. *et al*, *Acta Crystallogr.*, 1966, **20**, 301 (*cryst struct*)

$Al_2Be_2H_2Na_6O_{41}Si_{16}$ IC-000253
Leifite
[12417-54-8]

$Na_6Be_2[Al_2Si_{16}O_{39}](OH)_2.1.5H_2O$

M 1317.2
Open-branched, framework silicate. Mineral. Colourless cryst.

Coda, A. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 396 (*cryst struct*)

$Al_2Be_3O_{18}Si_6$ IC-000254
Beryl
[1302-52-9]

$Be_3Al_2[Si_6O_{18}]$

M 537.5
Unbranched single ring silicate; Si_6O_{18} rings are linked by AlO_6 octahedra and BeO_4 tetrahedra to form parallel channels which may occlude HCl. Mineral from USA, Canada, Colombia, Afghanistan, USSR etc. Gemstone: varieties incl. Emerald, Aquamarine, Goshenite, Heliodor, Morganite, Yorobyevite. Colourless, white, blue-green, green-yellow, yellow, blue cryst.

▷ DS1400000.

Solov'eva, L.N. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1966, **7**, 446 (*cryst struct*)
Morozin, B., *Acta Crystallogr., Sect. B*, 1972, **28**, 1899 (*cryst struct*)
Pavarennykh, A.S., *Mineral. Zh.*, 1979, **1**, 3 (*ir*)
Lehmann, G., *Phys. Chem. Miner.*, 1983, **9**, 278 (*esr*)
Magi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

$Al_2Bi_8Cl_9$ IC-000255
Octabismuth(2+) tetrachloroaluminate(1−) (1:2)
[81940-46-7]

$[Bi_8][AlCl_4]_2$

M 2009.4
Structure comprises $Bi_8^{2\oplus}$ square antiprisms and $AlCl_4^\ominus$ tetrahedra. Synth. from $Bi/BCl_3/AlCl_3$. Black moisture-sensitive cryst. (from melt). Mp 398°

Corbett, J.D. *et al*, *Inorg. Chem.*, 1968, **7**, 198 (*synth, str, phase diagram*)
Krebs, B. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 445 (*synth, cryst struct*)

$Al_2Br_7^\ominus$ IC-000256
μ-Bromohexabromodialuminate(1−)
Heptabromodialuminate(1−)

$[Br_3AlBrAlBr_3]^\ominus$ (C_2)

M 613.2 (ion)
K salt: [12284-89-8].
Al_2Br_7K M 652.3
Colourless v. moisture-sensitive cryst. (melt). Mp 196°. Complex with toluene descr.
Rb salt: [12284-90-1].
Al_2Br_7Rb M 698.7
Synth. from KBr-$AlBr_3$ melt. White moisture-sensitive solid. Forms a toluene solvate. Mp 110°.
Cs salt: [52564-85-9].
Al_2Br_7Cs M 746.1
Synth. from CsBr-$AlBr_3$ melt. White moisture-sensitive solid. Forms a toluene solvate. Mp 154°.
NH_4 salt: [56959-50-3].
$Al_2Br_7H_4N$ M 631.3
Synth. from Al_2Br_3 and NH_4Br. Colourless moisture sensitive cryst. (melt).

[52676-49-0]

Cronenberg, C.T.H.M. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **354**, 103 (*phase diagram, synth*)
Mikheeva, V.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 884 (*phase diagram*)
Begun, G.M. *et al*, *Inorg. Chem.*, 1971, **10**, 886 (*raman*)
Rytter, E. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 1541; 1975, **31**, 2177 (*cryst struct*)
Mikheeva, V.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1973, **22**, 2810 (*complexes*)
Deeg, T. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1975, **79**, 497 (*eqm*)
Weiden, N. *et al*, *Faraday Symp. R. Soc. Chem.*, 1978, **13**, 93 (*eqm*)
Dubois, B. *et al*, *C.R. Hebd. Seances Acad. Sci., Ser. 2*, 1981, **292**, 517 (*NMe_4 salt*)
Manteghetti, A. *et al*, *Spectrochim. Acta, Part A*, 1982, **38**, 141 (*ir, raman*)

$Al_2Ca_{0.5}H_{20}NaO_{34}Si_5$ IC-000257
Faujasite
Zeolite ZSM-3
[12173-28-3]

$NaCa_{0.5}[Al_2Si_5O_{14}].10H_2O$

M 641.5
Zeolite struct. FAU of hexagonal prisms, 14-hedra and 26-hedra with intersecting circular (740 pm dia.) channels in three dimensions, with$(Si,Al—O)_{12}$ rings. Some Si may be replaced by P or Ge; Al may be replaced by Ga. See also zeolites X and Y. Also formulated as $Na_{12}Ca_{12}Mg_{11}[(AlO_2)_{58}(SiO_2)_{134}]260H_2O$. Rare sedimentary mineral. Hydrothermal deposits in cavities of massive rocks, found in Germany, Switzerland and California. Synth. from Al_2O_3-SiO_2-Me_4NOH gels at 80°. Forms inclusion compds. with small molecules used in separation of gases. Important industrial catalyst, e.g. for isomerisation of alkylbenzenes; support for Wacker catalyst. White solid. Stable, reversible hydration. Void vol. 0.47cm^3 cm^{-3}. Hardness 5. Various ion exchanged forms known, (e.g. Ba, Cs, K, Na). Zeolite ZSM-20 has similar props.

Barrer, R.M. *et al*, *Proc. R. Soc. London, A*, 1958, **245**, 489 (*props*)
Barrer, R.M. *et al*, *Trans. Faraday Soc.*, 1957, **53**, 1111 (*adsorption hydrocarbons*)
Baur, W.H., *Am. Mineral.*, 1964, **49**, 697 (*cryst struct*)
U.S. Pat., 3 306 922, (1967); *C.A.*, **68**, 8434 (*synth*)
Kerr, G.T., *J. Phys. Chem.*, 1968, **72**, 2594 (*reactions*)
Aiello, R. *et al*, *J. Chem. Soc. A*, 1970, 1470 (*synth*)

Lerot, L. *et al*, *Mater. Res. Bull.*, 1974, **9**, 979 (*synth*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, New York, 1974, 143, 218
Barrer, R.M., *Hydrothermal Chemistry of Zeolites*, Academic Press, London, 1982
Giottardi, G. *et al*, *Natural Zeolites*, Springer, 1985, 214
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd., Butterworth, London, 1987, 62
de Saldarriaga, L.S. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 2686 (*Al-27, Si-29 and P-31 nmr*)
Ernst, S. *et al*, *Zeolites*, 1987, **7**, 180 (*ZSM-20*)
Ramamurthy, V. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 1213 (*use*)
Cormi, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 594 (*use*)
Espesi, P.H. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 669 (*use*)
Dwyer, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 905 (*Ga-substitution*)

IC-000258

$Al_2CaH_4O_{10}Si_2$
Lawsonite
[1318-81-6]

$CaAl_2[Si_2O_7](OH)_2.H_2O$

M 314.2
Mineral. Colourless or white rhombic cryst.
Baur, W.H., *Am. Mineral.*, 1978, **63**, 311 (*cryst struct*)
Chatterjee, N.D. *et al*, *Contrib. Mineral. Petrol.*, 1984, **88**, 1 (*synth*)

IC-000259

$Al_2CaH_8O_{20}Si_6$
Yugawaralite
[12343-47-4]

$Ca_2[Al_4Si_{12}O_{32}].8H_2O$

M 590.6
Member of phillipsite group. Zeolite struct. YUG with two sets of interconnected channels (280 × 360 and 310 × 500 pm across) each with $(Al,Si{-}O)_8$ rings. Some Ca replaced by Na or Sr. Mineral occurs in cavities of massive rocks. Found in India, Canada, Alaska and Japan. Hydrothermal synth. descr. White tubular cryst. ΔH_f° −9036 kJ mol^{-1}; ΔG_f° −8388 kJ mol^{-1}.
Barrer, R.M. *et al*, *Am. Mineral.*, 1965, **50**, 484 (*synth*)
Hawkins, D.B., *Mater. Res. Bull.*, 1967, **2**, 951 (*synth*)
Kerr, I.S. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 1183 (*cryst struct*)
Leimer, H.W. *et al*, *Z. Kristallogr.*, 1969, **130**, 88 (*cryst struct*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, Chichester, 1974 (*rev*)
Zeng, Y. *et al*, *Am. Mineral.*, 1982, **67**, 937 (*synth*)
Giottardi, G. *et al*, *Natural Zeolites*, Springer, Berlin, 1985, 110
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 138

$Al_2CaH_{24}O_{12}Si_4$ **IC-000260**
Levyne
Levynite (ingroper). ZK-20
[1318-83-8]

$Ca_6[Al_{12}Si_{24}O_{108}].30H_2O$

M 614.5
Zeolite struct. LEV with 17-hedron stacked in columns giving 2D network with channels (360 × 480 pm across) of $(Al,Si{-}O)_6$ rings. Member of chabazite group. Mineral of hydrothermal origin. Found in USA, Iceland, Japan, Italy and Australia. Hydrothermal synth. in presence of methylquinuclidine at 100°. White lamellae (melt). ZSM-20 similar.
Barrer, R.M. *et al*, *Trans. Faraday Soc.*, 1959, **55**, 1915 (*synth*)
U.S. Pat., 3 459 676, (1969); *CA*, **71**, 83105 (*synth*)
Kuhl, G.H., *Inorg. Chem.*, 1971, **10**, 2488 (*props*)
Wirsching, U., *Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Gottardi, G. *et al*, *Natural Zeolites*, Springer, Berlin, 1985, 192
Derouane, E.G. *et al*, *Appl. Catal.*, 1986, **28**, 285; 1988, **37**, 273 (*synth, powder data, Al-27, Si-29 nmr*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 78.
Dwyer, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 594 (*ir*)
Newsam, J.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 493 (*electron microgr*)
Thangaraj, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 493 (*N-14 nmr*)

IC-000261

Al_2CaO_4
Aluminium calcium oxide (Al_2CaO_4)
CA
[12042-68-1]

$CaAl_2O_4$

M 158.0
Stuffed tridymite struct. with Ca 6- or 9-coord. Used in ceramics and refractories and as support for transition metal and lanthanide phosphors. Commercially available. Microcryst. solid. Mp 1610°. ΔH_f° −2326.3 kJ mol^{-1} (298K); S° 114.2 J K^{-1} mol^{-1}. Related compds. $CaAl_{12}O_{20}$, $CaAl_4O_7$, $Ca_{12}Al_{14}O_{33}$ also descr.
Nurse, R.W. *et al*, *Trans. Brit. Ceram. Soc.*, 1965, **64**, 409 (*phase diagram*)
Tarte, P., *Spectrochim. Acta, Part A*, 1967, **23**, 2127 (*ir*)
Rao, M.R. *et al*, *J. Am. Ceram. Soc.*, 1968, **51**, 50 (*phase diagram*)
Palilla, F.C. *et al*, *J. Electrochem. Soc.*, 1968, **115**, 642 (*use*)
Kor, G.J.W. *et al*, *J. Iron Steel Inst., London*, 1968, **206**, 700 (*phase diagram*)
Brooksbank, D., *J. Iron Steel Inst., London*, 1968, **208**, 495 (*thermal exp*)
Oudalov, Y.P. *et al*, *Mater. Res. Bull.*, 1969, **4**, 887 (*synth*)
Imlach, J.A. *et al*, *Trans. Brit. Ceram. Soc.*, 1973, **72**, 221 (*system with FeO*)
Hörkner, W. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 983 (*cryst struct*)
Allibert, M. *et al*, *J. Am. Ceram. Soc.*, 1981, **64**, 307 (*thermodyn*)
Eliezer, I. *et al*, *J. Phys. Chem.*, 1981, **85**, 2835 (*thermodyn*)
Müller, D. *et al*, *J. Magn. Reson.*, 1984, **57**, 152 (*Al-27 nmr*)
Müller, D. *et al*, *Polyhedron*, 1986, **5**, 779 (*Al-27 nmr*)

$Al_2CaO_8Si_2$ **IC-000262**
Anorthite
Calcium aluminosilicate ($Ca(Al_2Si_2O_8)$)
[1302-54-1]

$Ca[Al_2Si_2O_8]$

M 278.2
Feldspar struct. with 3-D 4-connected net of AlO_4 and SiO_4 tetrahedra. Ca 6 or 7 coord. Identified in meteorites. Colourless to greyish or reddish cryst. Several modifications. Many minerals intermediate between this and Albite, IC-000224 are descr.
Takeuchi, Y. *et al*, *Acta Crystallogr.*, 1959, **12**, 465 (*cryst struct*)
Barrer, R.M. *et al*, *J. Chem. Soc.*, 1961, 983 (*synth*)
Kempster, C.J.E. *et al*, *Acta Crystallogr.*, 1962, **15**, 1005, 1017 (*cryst struct*)
Megaw, H.D. *et al*, *Acta Crystallogr.*, 1962, **15**, 1017.
Wainwright, J. *et al*, *Z. Kristallogr.*, 1971, **133**, 75 (*cryst struct*)
Takeuchi, Y. *et al*, *Z. Kristallogr.*, 1973, **137**, 380 (*cryst struct*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 4889 (*Si-29 nmr*)
Klinowski, J. *et al*, *J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Smith, K.A. *et al*, *Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)

$Al_2CaO_{12}Si_4$
Chabazite **IC-000263**
[12251-32-0]

$Ca(Al_2Si_4O_{12})$

M 398.3
Zeolite struct. CHA comprises columns of hexagonal prisms and 20 hedra giving rise to circular 3D channels 380 pm across of $(Si,Al{-}O)_8$ rings. Synth. from gel at 80°. Found as mineral in cavities in basalt, andesite, and other igneous rocks and as a recent deposit of certain hot springs (USA, Hawaii, Greenland, Ireland, Italy, Hungary, Australia, India, and elsewhere). White solid. Also known in various ion exchanged forms (Ag, K, Na, NH_4).
Barrer, R.M. *et al*, *J. Chem. Soc.*, 1956, 2882; 1964, 485 (*synth, K and Sr forms*)
Dent, L.S. *et al*, *Nature (London)*, 1958, **181**, 1794 (*cryst struct*)
Smith, J.V. *et al*, *Acta Crystallogr.*, 1963, **16**, 45.
Aiello, R. *et al*, *J. Chem. Soc. A*, 1970, 1470 (*synth*)
Wirsching, U., *Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4992; 1986, **108**, 1730 (*Al-27, Si-29 nmr*)
Fyfe, C.A. *et al*, *J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Pechar, F. *et al*, *Zeolites*, 1983, **3**, 333 (*ir*)
Nagy, J.B. *et al*, *Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Calligaris, M. *et al*, *Zeolites*, 1984, **4**, 251, 323; 1985, **5**, 317 (*cryst struct*)
Calligaris, M. *et al*, *Zeolites*, 1986, **6**, 137 (*cryst struct, Co, Ag forms*)

Al_2CaSe_4 **IC-000264**
Aluminium calcium selenide (Al_2CaSe_4)
Calcium diselenoxoaluminate(1−) (1:2)
[67847-61-4]

$CaAl_2Se_4$

M 409.8
Orthorhombic struct. has $AlSe_4$ tetrahedra sharing corners with $CaSe_8$ antiprisms. Struct. is related to TlSe. Synth. from elements at 1000°. Red, moisture-sensitive cryst.
Klee, W. *et al*, *Z. Naturforsch., B*, 1978, **33**, 829 (*cryst struct*)

$Al_2Ca_2FeHO_{13}Si_3$ **IC-000265**
Epidote, 9CI
Pistacite
[1318-49-6]

$Ca_2(Fe,Al)_3[SiO_4][Si_2O_7]O(OH)$ or $Ca_2[Al_2FeSi_3O_{12}(OH)]$

M 483.2
Mineral of the epidote group. If $Fe^{3\oplus}$ <15% (Fe + Al), the mineral is Clinozoisite. Mn replaces (Fe,Al) toward Piemontite. Struct. contains $[SiO_4]^{4\ominus}$ and $[Si_2O_7]^{2\ominus}$ with Al, Fe 6-coord. and Ca 8-coord. Common in contact zones and schists and an alteration product of feldspars. Minor gem stone. Yellowish green to brownish green prisms.
[11118-51-7]

Ito, T. *et al*, *Acta Crystallogr.*, 1954, **7**, 53 (*cryst struct*)
Dollase, W.A. *et al*, *Am. Mineral.*, 1971, **56**, 447 (*cryst struct*)
Gabe, E.J. *et al*, *Am. Mineral.*, 1973, **58**, 218 (*cryst struct*)
Deer, W.A. *et al*, *Rock Forming Minerals*, 2nd Ed., Longman, London, 1986, **1B**, 44 (*rev*)
Kvick, A. *et al*, *Acta Crystallogr., Sect. B*, 1988, **44**, 351 (*cryst struct*)

$Al_2Ca_2H_6O_{22}Si_6Sn$ **IC-000266**
Eakerite, 9CI
[12536-02-6]

$Ca_2Al_2Sn[Si_6O_{18}](OH)_2.2H_2O$

M 779.3
Mineral. The struct. contains crankshaft-like chains of composition $AlSi_3O_6(OH)$ which are cross-linked to form a kinked sheet. Occurs in spodumene-rich pegmatite in Cleveland County, North Carolina. Transparent monoclinic prisms.
Leavens, P.B. *et al*, *Mineral. Rec.*, 1970, **1**, 92 (*mineral*)
Kossiakoff, A.A. *et al*, *Am. Mineral.*, 1976, **61**, 956 (*cryst struct*)

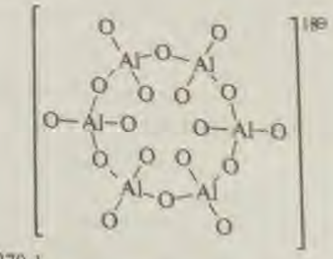
$Al_2Ca_3H_{12}O_{12}$ **IC-000267**
Aluminium calcium hydroxide ($Al_2Ca_3(OH)_{12}$)
[12291-41-7]

$Ca_3[Al(OH)_6]_2$

M 378.2
Struct. has $Al(OH)_6$ octahedra linked by H bonds with Ca dodecahedrally coordinated. 4OH may be replaced by SiO_4. Minerals $Ca_3Al_2(SO_4)_{3-x}(OH)_{4x}$ are known as Hydrogrossular or, for x = 1, Plazolite. Hydrothermal synth. from Al powder, CaO + H_2O at 100°. Colourless cryst. (aq. melt). Forms mixed cryst. with Grossular, IC-000269.
[12505-36-1]

Weiss, R. *et al*, *Acta Crystallogr.*, 1964, **17**, 1327 (*cryst struct*)
Cohen-Addad, C. *et al*, *J. Phys., (France)*, 1964, **25**, 478; *CA*, **61**, 11411 (*synth, pmr*)
Cohen-Addad, C. *et al*, *Acta Crystallogr.*, 1967, **23**, 220 (*cryst struct, ir, nd*)
Schwarz, H., *Z. Naturforsch., B*, 1967, **22**, 554 (*mixed cryst*)
Kuzel, H.J., *Neues Jahrb. Mineral., Monatsh.*, 1968, 87 (*mixed cryst*)

$Al_2Ca_3O_6$ **IC-000268**
Aluminium calcium oxide ($Al_2Ca_3O_6$)
C_3A_2
[12042-78-3]



M 270.1
Synth. by sudden chilling of CaO-Al_2O_3 melt from 1539°. Component of Portland cement. White cryst. (melt). Mp 1539°. Several similar compds. including hydrates descr. Reacts with water to give $2CaO.Al_2O_3.8H_2O$ <20° and $3CaO.Al_2O_3.6H_2O$ >20°. Dec. to CaO + liq. at 1535°. $\Delta H_{f\ 298}^\circ$ −3587.8 kJ mol^{-1}, S_{298}° 204.0 J K^{-1} mol^{-1}.
Weiss, R., *Adv. Chromatogr.*, 1964, **17**, 1329 (*hydrate*)
Nurse, R.W. *et al*, *Trans. Brit. Ceram. Soc.*, 1965, **64**, 409 (*phase diagram*)
Tarte, P., *Spectrochim. Acta, Part A*, 1967, **23**, 2127 (*ir*)
Kor, G.J.W. *et al*, *J. Iron Steel Inst., London*, 1968, **206**, 700 (*phase diagram*)
Brooksbank, D., *J. Iron Steel Inst., London*, 1968, **208**, 495 (*thermal exp*)

Imlach, J.A. *et al.* *Trans. Brit. Ceram. Soc.*, 1973, **72**, 221 (*system with PbO*)
Mondal, P. *et al.*, *6/10 Crystallogr., Suec. R*, 1973, **31**, 689 (*cryst struct*)
Allibert, M. *et al.*, *J. Am. Ceram. Soc.*, 1981, **64**, 307 (*thermodyn*)
Ellner, I. *et al.*, *J. Phys. Chem.*, 1981, **85**, 2855 (*thermodyn*)
Miller, H. *et al.*, *Polyhedron*, 1986, **5**, 779 (*Al-27 nmr*)

IC-000269

$Al_2Ca_3O_{12}Si_3$
Grossular
Grossularite
[1302-57-4]

$Al_2Ca_3(SiO_4)_3$

M 450.4
Garnet struct. in which AlO_6 octahedra and SiO_4 tetrahedra share corners. Dodecahedral coordn. at Ca. Often contains $Fe^{3\oplus}$ replacing Ca, and $Fe^{3\oplus}$ replacing Al. Mineral occurs as metamorphosed impure calcareous rock, especially in contact zones. Widespread in western USA, also found in Canada, Italy, USSR, Korea, Australia, Sri Lanka and Switzerland. Colourless cryst. (impurities give grey, yellow, green, brown, black cryst.) SiO_4 may be replaced by 4 OH to give hydrogarnets. $Al_2Ca_3(SiO_4)_3(OH)_{12}$. See Aluminium calcium hydroxide $[Al_2Ca_3(OH)_{12}]$. IC-000267.

Abrahams, S.C. *et al.* *Acta Crystallogr.*, 1958, **11**, 437 (*cryst struct*)
Barrer, R.M. *et al.*, *J. Chem. Soc.*, 1961, 983 (*synth*)
Prandl, W., *Z. Kristallogr.*, 1966, **123**, 81 (*cryst struct, ref*)
Colani Addad, *et al.*, *Acta Crystallogr.*, 1967, **23**, 220 (*cryst struct*)
Hazen, R.M. *et al.*, *Am. Mineral.*, 1978, **63**, 297 (*cryst struct*)
Deer, W.A. *et al.*, *Rock Forming Minerals*, 2nd Ed., Longman, London, 1982, **1A**, 603 (*rev*)

IC-000270

Al_2CdCl_8
Cadmium bis(tetrachloroaluminate)
Tetra-μ-chlorobis(dichloroaluminium)cadmium
[13138-81-5]

$Cd[AlCl_4]_2$

M 449.9
Formed in a melt of $CdCl_2$ + $AlCl_3$. Colourless cryst. Mp 208°.

Staffel, T. *et al.*, *Z. Anorg. Allg. Chem.*, 1987, **548**, 45 (*synth, cryst struct*)

IC-000271

Al_2CdO_4
Aluminium cadmium oxide (Al_2CdO_4)
[12252-16-3]

$CdAl_2O_4$

M 230.3
Partly inverted spinel. Synth. from CdO + $Al(OH)_3$ at 800°. Brown solid. Thermal expansion 2.81×10^{-6} K^{-1}.

Hahn, H. *et al.*, *Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*phase diagram*)
Colin, F. *et al.*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1966, **263**, 1220 (*powder struct, ref compds*)
Navrotsky, A. *et al.*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 479 (*synth, thermodyn data*)
Huseby, I.C. *et al.*, *Am. Ceram. Soc. Bull.*, 1981, **60**, 919 (*thermal props*)
Otero, A.C. *et al.*, *CA*, 1981, **94**, 98038 (*cryst struct*)

IC-000272

Al_2CdS_4
Aluminium cadmium sulfide (Al_2CdS_4)
[12359-70-5]

$CdAl_2S_4$

M 294.6
Low pressure phase has tetragonal $CdGa_2S_4$ struct., 3-coord. S are ccp and Al and Cd are tetrahedral. Spinel form obt. at high pressure and temp. Synth. from Al + CdS. Brown solid. Band gap 3.2 eV.

Hahn, H. *et al.*, *Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)
Range, K.J. *et al.*, *Z. Naturforsch., B*, 1968, **23**, 1009 (*high press form*)

IC-000273

Al_2CdSe_4
Aluminium cadmium selenide (Al_2CdSe_4)
[12359-71-6]

$CdAl_2Se_4$

M 482.2
Low pressure phase has tetragonal $CdGa_2S_4$ struct., 3-coord. S are ccp and Cd, Al are tetrahedral. Spinel formed at black high pressure and temp. Synth. from Al_2Se_3 and CdSe. Black solid. Band gap 2.5 eV.

Hahn, H. *et al.*, *Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)
Range, K.J. *et al.*, *Z. Naturforsch., B*, 1968, **23**, 1009 (*cryst struct*)

IC-000274

Al_2CdTe_4
Aluminium cadmium telluride (Al_2CdTe_4)
[12421-31-7]

$CdAl_2Te_4$

M 676.7
Various modifications descr. including tetragonal $CdGa_2S_4$ struct. in which 3-coord. Te are ccp and Cd, Al are tetrahedral. Synth. from Al_2Te_3 and CdTe. Black solid.

Hahn, H. *et al.*, *Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)
Chizhikov, V.I. *et al.*, *Phys. Status Solidi B*, 1981, **106**, 91 (*electrical props*)

IC-000275

$Al_2Cd_2Cl_8$
Cadmium(I) tetrachloroaluminate ($Cd_2(AlCl_4)_2$)
Dicadmium(2+) bis(tetrachloroaluminate(1−)). Aluminium cadmium chloride ($Al_2Cd_2Cl_8$)
[79110-87-5]

$Cd_2(AlCl_4)_2$

M 562.4
Struct. comprises slabs, stacked in [100] direction, consisting of ethane-like Cd_2Cl_6 units, sharing common vertices with $AlCl_4$ tetrahedra. Synth. from $Cd(AlCl_4)_2$ and excess Cd. V. moisture-sensitive colourless cryst. Dec. at 227° to Cd and $Cd(AlCl_4)_2$. Disproportionates in solvs. more basic than C_6H_6.

Corbett, J.D. *et al.*, *J. Am. Chem. Soc.*, 1961, **83**, 76 (*synth, powder struct*)
Corbett, J.D., *Inorg. Chem.*, 1962, **1**, 700 (*raman*)
Staffel, T. *et al.*, *Z. Anorg. Allg. Chem.*, 1987, **548**, 45 (*synth, cryst struct*)

$Al_2Cl_7^{\ominus}$ IC-000276
μ-Chlorohexachlorodialuminate(1−)
Heptachlorodialuminate(III)
[27893-52-3]

$[Cl_3AlClAlCl_3]^{\ominus}$

M 302.1 (ion)
$Al_3Cl_{10}^{\ominus}$ also descr.
Hexa-μ-chlorotris[(1,2,3,4,5,6-η)-hexamethylbenzene] trizirconium(2+) salt (2:1): [79153-33-6]. From C_6Me_6, $AlCl_3$ and $ZrCl_4$ in C_6H_6. Brown-black air- and moisture-sensitive cryst.
Acetyl salt:
$C_2H_3Al_2Cl_7O$ M 345.1
White moisture-sensitive solid.
$[Te_4]^{2\oplus}$ salt: see *Cyclotetratellurium(2+), IC-021993*

Peach, M.E. *et al.*, *J. Chem. Soc. A*, 1969, 366 (*ir*)
Cyvin, S.J. *et al.*, *J. Chem. Phys.*, 1970, **52**, 2776 (*ir, raman*)
Couch, T.W. *et al.*, *Inorg. Chem.*, 1972, **11**, 351 (*cryst struct*)
Fannin, A.A. *et al.*, *J. Electrochem. Soc.*, 1972, **119**, 801 (*electrochem*)
Jens, H. *et al.*, *Inorg. Chem.*, 1973, **12**, 1891 (*electrochem*)
Boxall, L.G. *et al.*, *J. Electrochem. Soc.*, 1973, **120**, 223 (*thermodyn data*)
Rytter, E. *et al.*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1185 (*raman*)
Ikeuchi, H. *et al.*, *Acta Chem. Scand., Ser. A*, 1974, **28**, 48 (*electrochem*)
Merryman, D.J. *et al.*, *Inorg. Chem.*, 1974, **13**, 1471 (*nqr*)
Gale, R.J. *et al.*, *Inorg. Chem.*, 1978, **17**, 2728 (*raman*)
Stollmaier, F. *et al.*, *J. Organomet. Chem.*, 1981, **208**, 327 (*cryst struct*)
Morozov, A.I. *et al.*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 186 (*ir*)
Manteghetti, A. *et al.*, *Spectrochim. Acta, Part A*, 1982, **38**, 141 (*ir, raman*)
Hussey, C.L., *Adv. Molten Salt Chem.*, 1983, **5**, 185 (*rev*)
Abdul-Sada, A.K. *et al.*, *Org. Mass Spectrom.*, 1989, **24**, 917 (*ms*)

Al_2Cl_8Cu IC-000277
Copper(II) tetrachloroaluminate ($Cu(AlCl_4)_2$)
Copper(2+) bis[tetrachloroaluminate(1−)]. Di-μ-chlorochloro(μ-chlorotetrachlorodialuminium)copper
[58915-60-9]

$Cu(AlCl_4)_2$

M 401.1
In cryst. $AlCl_4$ tetrahedra share edges and corners with tetragonally distorted $CuCl_6$ octahedra. Synth. from $AlCl_3$ and $CuCl_2$ by chemical transport at 170-230°. Catalyst for isom. of pentane. Blue prismatic moisture-sensitive cryst.
[67607-15-2]

Schläpfer, C.W. *et al.*, *Inorg. Chem.*, 1978, **17**, 1623 (*raman*)
Schäfer, H. *et al.*, *Z. Anorg. Allg. Chem.*, 1980, **461**, 31 (*synth, cryst struct*)
Ono, Y. *et al.*, *J. Mol. Catal.*, 1981, **10**, 121 (*use*)
Kitajima, N. *et al.*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 2064 (*synth, cryst struct*)

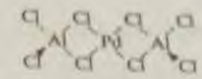
$Al_2Cl_8Hg_3$ IC-000278
Trimercury(2+) bis[tetrachloroaluminate(1−)]
[36554-82-2]

$Cl_3Al{-}Cl{-}HgHgHg{-}Cl{-}AlCl_3$

M 939.3
Molecular struct. in solid state. Obt. from $HgCl_2$, Hg and $AlCl_3$ (1:2:2) at 200-250°. Yellow highly hygroscopic needles (melt). Mp 203-205°.

Torsi, G. *et al.*, *Inorg. Chem.*, 1971, **10**, 2285 (*synth, raman, electrochem*)
Ellison, R.D. *et al.*, *Inorg. Chem.*, 1972, **11**, 833 (*synth, cryst struct*)
Merryman, D.J. *et al.*, *Inorg. Chem.*, 1974, **13**, 1471 (*nqr*)

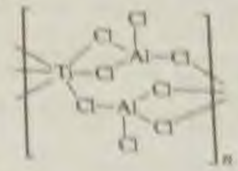
Al_2Cl_8Pd IC-000279
Palladium(II) tetrachloroaluminate ($Pd(AlCl_4)_2$)
Tetra-μ-chlorobis(dichloroaluminium)palladium, 9CI
[40556-05-6]



M 444.0
Molecular struct. in solid state: square planar $PdCl_4$ units share edges with $AlCl_4$ tetrahedra. Synth. from $PdCl_2$ and $AlCl_3$ at 180°. Dark red needles and plates (vapour). Corresp. Pt compd. also descr.

Papatheodorou, G.N., *J. Phys. Chem.*, 1973, **77**, 472 (*synth, struct, thermodyn data*)
Papatheodorou, G.N., *Inorg. Nucl. Chem. Lett.*, 1974, **10**, 115 (*synth, powder struct, magnetism*)
Schäfer, H. *et al.*, *Z. Anorg. Allg. Chem.*, 1981, **478**, 37 (*ms, Pt compd*)
Lenhard, W. *et al.*, *Z. Anorg. Allg. Chem.*, 1981, **482**, 19 (*synth, cryst struct*)

Al_2Cl_8Ti IC-000280
Tetra-μ-chlorobis(dichloroaluminium)titanium(II), 11Cl
Aluminium titanium chloride (Al_2TiCl_8), 10Cl. Titanium bis[tetrachloroaluminate(1−)]
[84556-32-1]



M 385.4
Polymeric. Can be oxidised electrochemically to Ti(III), then Ti(IV) in NaCl/$AlCl_3$ melts.

α-form
Chain struct. comprising hcp chlorine with Ti in O_h sites and Al in T_d sites in every other layer. Synth. from $AlCl_3$ and Ti metal at 225° for 1 month in a sealed quartz tube. Greenish-blue needles. Sol. hot C_6H_6, forming solvate.
▷ Potentially hazardous synth.

β-form
Synth. from α-form by subl. at 230-240° in a sealed quartz tube. Green cryst.

C_6H_6 solvate (1:1): [12312-06-0].
Synth. by adding a soln. of $TiCl_4$ in C_6H_6 to the product of heating Al + $AlCl_3$ to 140°, or by dissolving the α-form in C_6H_6 at 70° and slowly cooling to r.t. Catalyses alkylation of aromatics and polym. of α-olefins. Violet cryst. (C_6H_6).

Toluene solvate (1:1): [12287-52-4].
Synth. by reduction of $TiCl_4$ with Al + $AlCl_3$ in toluene. Catalyses cyclotrimerisation of butadiene, alkylation of aromatics and polym. of α-olefins. Violet solid (toluene).

[12726-00-0, 31174-61-3]

Fr. Pat., 1 460 233, (1966); *CA*, **67**, 11928t (*use*)
U.S. Pat., 3 374 279, (1968); *CA*, **68**, 106638h (*use*)

Bryenstad, J. et al., Inorg. Nucl. Chem. Lett., 1970, 6, 880 (synth, cryst struct, ir-vis)
Fung, K.W. et al., J. Electroanal. Chem. Interfacial Electrochem., 1972, 35, 27 (electrochem)
Pszeniczek, S. et al., J. Organomet. Chem., 1973, 54, 203, 1975, 87, 293 (synth, deriv)
Dziewiszowski, S. et al., J. Mol. Catal., 1977, 2, 243 (use)
Isotani, A. et al., Polyhedron, 1982, 1, 793 (synth, ir, w- and fl-forms, sol)

IC-000281

Al_2CoO_4

Aluminium cobalt(II) oxide (Al_2CoO_4)

[1333-88-6]

$CoAl_2O_4$

M 176.8
A spinel. Synth. from CoO and Al_2O_3 at 1200°. Oxidation and desulfurisation catalyst. Pigment in photography and with ZnS phosphors. Commercially available.

Tarte, P., Spectrochim. Acta, Part A, 1967, 23, 2127 (ir)
Yaremisky, A. et al., J. Inorg. Nucl. Chem., 1968, 30, 479 (synth, props)
Dutz, R.V. et al., J. Am. Ceram. Soc., 1975, 58, 462 (thermodyn, props)
Otero, A.C. et al., CA, 1981, 94, 94058 (cryst struct)

IC-000282

Al_2CrS_4

Aluminium chromium sulfide (Al_2CrS_4)

Chromium thioaluminate

[12516-10-6]

Al_2CrS_4

M 234.2
A spinel. Synth. from H_2S + Cr/Al or CrS/Al mixts. at 1250-1350°. Black cryst.

Flahaut, J., Ann. Chim. (Paris), 1952, 7, 632 (synth)
Flahaut, J. et al., Compt. Rend. Hebd. Seances Acad. Sci., 1961, 253, 1956 (synth, struct)
Tremayne, S.L.D. et al., J. Solid State Chem., 1977, 20, 345 (thermodynamics)

IC-000283

Al_2EuSe_4

Aluminium europium selenide (Al_2EuSe_4)

[11078-17-8]

Al_2EuSe_4

M 521.7
Prepd. by heating EuSe, Al and Se mixts. Cryst. Paramagnetic at 80-300K.

Blasse, G. et al., Bull. Soc. Chim. Fr., 1971, 747 (synth, cryst struct, magnetism)

IC-000284

$Al_2FeH_4O_{10}Si_2$

Ferrierpholite

[12321-46-7]

$FeAl_2[Si_2O_7](OH)_2$

M 330.0
Unbranched, single chain silicate (2 SiO_4 units per chain). Also formulated as $(Fe,Mg)Al_2Si_2O_7(OH)_2$. Mineral. Dark green to grey cryst.

MacGillavry, C.H. et al., Acta Crystallogr., 1950, 3, 272 (cryst struct)
Viswanathan, K. et al., Compt. Mineral. Petrol., 1978, 76, 45 (cryst struct)
Viswanathan, K., Am. Mineral., 1981, 66, 1000 (cryst struct)

Al_2FeO_4

Iron(II) aluminate ($FeAl_2O_4$)

[12068-49-4]

$FeAl_2O_4$

M 173.8
Spinel struct. Present in blast furnace slag. Formed at ceramic-steel interface. Absorbent for H_2S. Catalyst e.g. for oxidation of chloroethane waste gases. Component of coatings on glass-ceramics. Used in humidity sensors and in iron catalysts for NH_3 manuf. Solid.

Mineral-form [1302-61-0]
Hercynite
Black, opaque cryst.

Dickson, B.L. et al., Can. Mineral., 1976, 14, 206 (mössbauer)
Knapp, G.S. et al., Solid State Commun., 1982, 44, 1343 (xanes)
Hill, R.J., Am. Mineral., 1984, 69, 937 (struct)
Lenglet, M. et al., Rev. Chim. Miner., 1987, 24, 81 (xanes, uv-vis)

IC-000286

Al_2FeS_4

Aluminium iron sulfide (Al_2FeS_4)

Iron thioaluminate

[39368-30-4]

Al_2FeS_4

M 238.0
Prepd. by heating Al + FeS + excess S to 140°. Also formed in the sulfidation of Fe/Al alloys. Cryst. Easily hydrol.

Flahaut, J., Ann. Chim. (Paris), 1952, 7, 632 (synth)
Nishida, K. et al., CA, 1977, 86, 82926u (synth)
Petrasik, P.C. et al., J. Electrochem. Soc., 1985, 132, 1226 (formn)

IC-000287

$Al_2Fe_3O_{12}Si_3$

Aluminium iron(II) silicate ($Al_2Fe_3(SiO_4)_3$)

Almandine. Almandite. Dialumunium triiron trisilicate

[1302-62-1]

$Al_2Fe_3(SiO_4)_3$

M 497.7
Mineral of the garnet group. Occur. widespread, esp. in metamorphic rocks. For synthetic garnets. Deep red to brown. Transparent. Vitreous to resinous.

Roberts, W.L. et al., Encyclopedia of Minerals, Van Nostrand, 1974 (rev)
Andreu, M.A., Gemologia (Barcelona), 1974, 6, 51 (gemstone)
Hunt, G.R., Geophysics, 1977, 42, 501 (ir)
Parkin, K.M. et al., Geochim. Cosmochim. Acta, Suppl., 1980, 14, 731 (uv-vis, use)
Kieffer, S.W., Rev. Geophys. Space Phys., 1980, 18, 862 (thermodyn, props)
Barriskill, R.L., CA, 1981, 95, 228354r (struct, bonding)
Aines, R.D. et al., Am. Mineral., 1984, 69, 1116 (ir, water content)
Smith, G. et al., CA, 1984, 100, 42175z (use)
Waychunas, G.A. et al., Phys. Chem. Miner., 1986, 13, 31 (exafs, struct)

IC-000288

$Al_2H_2Mg_2Na_{24}Si_8$

Glaucophane

[12173-39-6]

$Na_2Mg_3Al_2[Si_8O_{11}]_2(OH)_2$

M 783.5
Monoclinic. Unbranched, double chain silicate. Mineral. Grey or lavender blue cryst. Also formulated as $Na_2(Mg,Fe)_3Al_2[Si_8O_{11}]_2(OH)_2$ and $Al_2Mg_3Na_2H_2(SiO_3)_8$.

[61158-93-8]
Papike, J.J. et al., Am. Mineral., 1968, 53, 1156 (cryst struct)
Maliuski, H. et al., Bull. Soc. Geol. Fr., 1981, 23, 401
Hoffmann, C. et al., Lithos, 1982, 15, 17
Valizer, P.M. et al., Mineral. Issled. Endog. Mestorozhd. Urala, 1982, 118; CA, 1983, 99, 8374 (ir)
Liu, W. et al., Kexue Tongbao (Foreign Lang. Ed.), 1986, 31, 483; CA, 105, 63847p (em)

IC-000289

$Al_2H_2O_{12}Si_4$

Pyrophyllite

[12269-78-2]

$Al_2Si_4O_{10}(OH)_2$

M 360.3
Struct. has double layers each comprising AlO_6 octahedra between 2 layers of SiO_4 tetrahedra. Mineral. Used in pigments, ceramics, binders and adsorbents. White to grey solid.

Hassanein, M. et al., Z. Anorg. Allg. Chem., 1968, 356, 321 (reactions)
Van Olphen, H. et al., Introduction to Clay Colloid Chemistry, 2nd Ed., Wiley, 1977, 63.
Lippmaa, E. et al., J. Am. Chem. Soc., 1980, 102, 4889 (Si-29 nmr)
Smith, K.A. et al., Am. Mineral., 1983, 68, 1206 (Si-29 nmr)
Sanz, J. et al., J. Am. Chem. Soc., 1984, 106, 4790 (Si-29, Al-27 nmr)
Mägi, M. et al., J. Phys. Chem., 1984, 88, 1518 (Si-29 nmr)
Kinsey, R.A. et al., Am. Mineral., 1985, 70, 537 (Al-27, Si-29 nmr)

IC-000290

$Al_2H_4I_2O_{14}Si_4$

Bikitaite

[12003-53-1]

$Li_2[Al_2Si_4O_{12}].2H_2O$

M 408.2
Zeolite struct. BIK, member of mordenite group. Struct. comprises puckered sheets of Al/SiO_4 tetrahedra linked through single tetrahedral chains giving 1D channels of 280 × 370 pm across. Mineral found in Li-rich pegmatites in Zimbabwe and North Carolina. Synth. from LiOH, $Al(OH)_3$ + H_2O at 300-350° and 2000 atm. Colourless cryst. Void fraction 0.23 $cm^3\ cm^{-3}$. Loses 7.5% H_2O at 230°.

Appleman, D.E., Acta Crystallogr., 1960, 13, 1002 (cryst struct)
Dryzdale, D.J., Am. Mineral., 1971, 56, 1718 (synth)
Breck, D.W., Zeolite Molecular Sieves, Wiley, N.Y., 1973, 136, 210, 259 (synth, props)
Kocman, V. et al., Am. Mineral., 1974, 59, 71 (cryst struct)
Bissert, G. et al., Neues Jahrb. Mineral., Monatsh., 1986, 241; CA, 105, 9396.
Meier, W.M. et al., Atlas of Zeolite Structure Types, 2nd Ed., Butterworth, London, 1987, 36.

IC-000291

$Al_2H_4Mg_2O_9Si$

Amesite, 9CI

[12413-43-3]

$Mg_2[Al_2O_3(SiO_4)].2H_2O$

M 278.6
Rare mineral. A septechlorite of the serpentine group. A 1:1 layer silicate with the maximum amount of tetrahedral and octahedral Al-substitution. Often contains Fe. Also formulated as $Mg_2Al(Si,Al)O_5(OH)_4$. First recorded at Chester, Mass, USA, also found in USSR and Canada. Pure compd. obt. by acid treatment of mineral at 550°. Pale green, translucent hexagonal plates.

Brindley, G.W. et al., Acta Crystallogr., 1951, 4, 552 (cryst struct, thermal decr)
Steinfink, H. et al., Acta Crystallogr., 1956, 9, 487 (cryst struct)
Deer, W.A. et al., Rock Forming Minerals, 2nd Ed., Longmans, London, 1962, 3, 166 (rev)
Hall, S.H. et al., Am. Mineral., 1976, 61, 497 (occur)
Anderson, C.S. et al., Am. Mineral., 1981, 66, 187 (cryst struct)
Serna, C.J. et al., Am. Mineral., 1982, 67, 1095 (ir)

IC-000292

$Al_2H_4MnO_{10}Si_2$

Carpholite

[12246-88-7]

$MnAl_2[Si_2O_6](OH)_4$

M 329.0
Unbranched single chain silicate. Mineral; occurs in Belgium, Czechoslovakia, USSR, Yugoslavia and Germany. Fibrous or prismatic, golden yellow, colourless or yellow tinted cryst.

Lindemann, W. et al., Neues Jahrb. Mineral., Monatsh., 1979, 281 (cryst struct)
Viswanathan, K., Am. Mineral., 1981, 66, 1090 (cryst struct)

IC-000293

$Al_2H_4Na_2O_{12}Si_3$

Natrolite

[1318-95-2]

$Na_{16}[Al_{16}Si_{24}O_{80}].16H_2O$

M 380.2
Zeolite struct. NAT with 2D channels (260 × 390 pm across) of $(Al,Si—O)_8$ rings interconnected with 1D channels of variable dia. $(Al,Si—O)_8$ rings. Mineral. Difficult to obtain by laboratory methods but of widespread occurrence in natural hydrothermal deposits. Fibrous white cryst. Related minerals: Mesolite and Scolecite also descr.

Meier, W.M., Z. Kristallogr., 1960, 113, 430 (cryst struct)
Petch, H.E. et al., J. Chem. Phys., 1962, 36, 1216 (Na-23, Al-27 nqr)
Peacor, D.R., Am. Mineral., 1973, 58, 676 (cryst struct)
Fälth, L. et al., Acta Crystallogr., Sect. B, 1979, 35, 1877 (cryst struct)
Lippmaa, E. et al., J. Am. Chem. Soc., 1980, 102, 4889, 1981, 103, 4992, 1986, 108, 1730 (Si-29, Al-27 nmr)
Alberti, A. et al., Acta Crystallogr., Sect. B, 1981, 37, 781 (cryst struct)
Wüsching, U., Clays Clay Miner., 1981, 29, 171 (synth, powder struct)
Artioli, G. et al., Acta Crystallogr., Sect. C, 1984, 40, 1658 (ind)
Kirfel, A. et al., Zeolites, 1984, 4, 140 (cryst struct)
Jaros, N. et al., J. Am. Chem. Soc., 1985, 107, 6760 (Si-29 nmr)
Gottardi, G. et al., Natural Zeolites, Springer-Verlag, 1985, 35 (props)
Artioli, G. et al., Acta Crystallogr., Sect. C, 1986, 42, 937 (cryst struct, mesolite)
Meier, W.M. et al., Atlas of Zeolite Structure Types, 2nd Ed., Butterworth, London, 1987, 110.

IC-000294

$Al_2H_4O_7Si$

Imogolite

[12263-43-3]

$(HO)_3Al_2O_3Si(OH)$

M 198.0
Struct. comprises gibbsite sheet closed to form tube of ca. 2300 pm diameter and 10^4 - 10^7 pm long. Internal channel (ca. 820 pm across) normally occupied by H_2O. Variety of Allophane. Mineral widely distributed in

volcanic deposits. Formed from dil. soln. cont. Al and Si at pH 3.5–5. Possible catalyst for dehydration of alcohols. White solid. Forms pillared intercalation compd. with Na montmorillonite.

Farmer, V.C. *et al, Clay Miner.*, 1977, **12**, 55 (*ir*)
Farmer, V.C., *J. Chem. Soc., Chem. Commun.*, 1977, 462 (*synth*)
Barron, P.F. *et al, Nature (London)*, 1982, **299**, 616 (*Si-29 nmr*)
Wilson, M.A. *et al, J. Soil Sci.*, 1984, **35**, 201; *Anal. Chem.*, 1985, **57**, 2733 (*Al-27, Si-29 nmr, anal*)
Goodman, B.A. *et al, Phys. Chem. Miner.*, 1985, **12**, 342 (*Si-29, Al-27 nmr*)
Johnson, I.D. *et al, J. Am. Chem. Soc.*, 1988, **110**, 8545 (*synth, Si-29 nmr, props*)

IC-000295

$Al_2H_4O_9Si_2$
Kaolinite, 9Cl
[1318-74-7]

$Al_2[Si_2O_5](OH)_4$

M 258.1
Mineral of the Kaolin group. Trimorphous with Dickite and Nacrite, IC-000296 with single kaolin layers each with hexagonal net of SiO_4 tetrahedra and $Al(O,OH)_6$ octahedra. V. common clay mineral. Formed by the hydrothermal alteration or weathering of other aluminosilicates. Filler in paper, rubber, paints, etc.; ceramic and refracting raw material; whitening agent in textiles and paper. White to grey hexagonal platelets. Amorphous dehydrated form (Metakaolinite) also descr. Cation exchange capacity 0.03–0.15 eq kg^{-1}.

Zvyagin, V.V., *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1960, **5**, 32 (*cryst struct*)
Deer, W.A. *et al, Rock-Forming Minerals*, Longman, London, 1962, **3**, 194 (*rev*)
Barrer, R.M. *et al, J. Chem. Soc. A*, 1968, 2475; 1974, 934 (*reactions*)
Van Olphen, H., *Clay Colloid Chemistry*, Wiley, 2nd Ed., 1977 (*rev, props*)
Bullens, M. *et al, J. Am. Ceram. Soc.*, 1978, **61**, 81 (*esco, fluorescence*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **3**, 190, 207; **5**, 238; **6**, 195, 208 (*rev, uses*)
Mägi, M. *et al, J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)
Kinsey, R.A. *et al, Am. Mineral.*, 1985, **70**, 537 (*Al-27, Si-29 nmr*)
Engelhardt, G. *et al, High Resolution Solid State NMR of Silicates and Zeolites*, Wiley, Chichester, 1987 (*Si-29, Al-27 nmr*)
Bailey, S.W., *Clays Clay Miner.*, 1988, **36**, 193 (*identification*)
Giese, R.F. *et al, Rev. Mineral.*, 1988, **19**, 29 (*rev*)
Rocha, J. *et al, J. Chem. Soc., Chem. Commun.*, 1991, 582 (*Al-27, Si-29 nmr*)

$Al_2H_4O_9Si_2$ IC-000301
Dickite
[1318-45-2]

$Al_2[Si_2O_5](OH)_4$

M 258.2
Clay mineral with sequence of two kaolin layers each with hexagonal net of SiO_4 tetrahedra and $Al(O,OH)_6$ octahedra. From Al_2O_3–SiO_2–H_2O gels at 300°. Occurs as hydrothermal mineral in USA, USSR and Japan. Flaky white cryst.

Newnham, R.E. *et al, Acta Crystallogr.*, 1956, **9**, 759 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **3**, 195, 207; **5**, 238; **6**, 195, 208 (*rev, uses*)
Barrer, R.M., *Hydrothermal Chemistry of Zeolites*, Academic Press, London, 1982, 78 (*synth*)
Bailey, S.W., *Clays Clay Miner.*, 1988, **36**, 193 (*identification*)

$Al_2H_4O_9Si_2$
Nacrite
[12279-65-1]

$Al_2Si_2O_5(OH)_4$

M 258.1
Natural clay with sequence of 6 kaolin layers each with hexagonal net of SiO_4 tetrahedra and $Al(O,OH)_6$ octahedra. Rare mineral. Flaky white monoclinic cryst. Hydrated form with H_2O between layers also descr.

Newnham, R.E. *et al, Acta Crystallogr.*, 1956, **9**, 759 (*cryst struct*)
Van Olphen, H., *Clay Colloid Chemistry*, 2nd Ed., Wiley, N.Y., 1977 (*rev, props*)
Barrer, R.M., *Hydrothermal Chemistry of Zeolites*, Academic Press, London, 1982, 78 (*synth*)

IC-000297

$Al_2H_6O_7^{2\ominus}$
Aluminate ($Al_2(OH)_6O^{2\ominus}$)
Hexahydroxy-μ-oxodialuminate(2−)
[54968-30-8]

$[(HO)_3AlOAl(OH)_3]^{2\ominus}$

M 172.0 (ion)
Di-K salt: [12043-00-4].
$Al_2H_6K_2O_7$ M 250.2
Synth. from Al and KOH. Colourless cryst. (H_2O). V. sol. H_2O; spar. sol. EtOH.
Di-Rb salt: [74848-20-7].
$Al_2H_6O_7Rb_2$ M 342.9
Synth. from Al and RbOH. Colourless cryst. (H_2O).
Cs salt: [77011-52-0].
$Al_2Cs_2H_6O_7$ M 437.8
Synth. from Al + CsOH. Colourless cryst. (H_2O).

[50989-46-3]

Johansson, G., *Acta Chem. Scand.*, 1966, **20**, 505 (*synth, cryst struct*)
Haladjian, J. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 3821 (*ir, raman*)
Ivlieva, V.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 1107 (*synth, powder struct*)
Ivanov Emin, B.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 295, 1661 (*synth, phase diagram, powder struct*)

$Al_2H_7LiO_7$ IC-000298
Aluminium lithium hydroxide ($Al_2Li(OH)_7$)
Lithium dialuminate

$[LiAl_2(OH)_6](OH)$

M 179.9
Dihydrate [12344-53-5].
$Al_2H_{11}LiO_9$ M 215.9
From LiOH, H_2O, $Al(OH)_3$ and H_2O vapour. Less pure samples by precipitation from aq. soln. White solid. Converts on heating to $LiAlO_2$. Related compds. with one OH replaced by Cl, Br, I, BO_3, H_2PO_4, NO_3 also descr. Struct. comprises sheets as in Aluminium hydroxide ($Al(OH)_3$), IC-000179 with replacement of one third of Al by Li and $OH^\ominus$, H_2O between.

Lileev, I.S. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 213 (*synth*)
Miyata, S., *Clays Clay Miner.*, 1975, **23**, 369 (*synth, rel compds*)
Ashchyan, T.O. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 74, 341 (*synth, rel compds*)
Serna, C. *et al, Clays Clay Miner.*, 1982, **30**, 180 (*ir*)
Poppelmeier, K.R. *et al, Inorg. Chem.*, 1987, **26**, 3297 (*synth, powder struct, rel*)

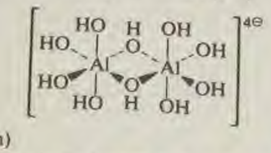
$Al_2H_8Mg_5O_{18}Si_3$ IC-000299
Chlorite
Prochlorite
[1318-59-8]

$[Mg_2Al(OH)_6][Mg_3(AlSi_3O_{10})(OH)_2]$

M 555.7
Typical formula given. Class of clay mineral with alternate positively and negatively charged layers; Si tetrahedrally and Mg,Al octahedrally coord. There are two types: trioctahedral chlorite has $Mg_{6-x-y}Fe_y^{2\oplus}Al_x(Si_{4-x}Al_x)O_{10}(OH)_8$ and dioctahedral chlorite $(Al_{4+x/3})(Si_{4-x}Al_x)O_{10}(OH)_8$. Occurs widely as mineral. Used in ceramic manuf. and as a catalyst support. White to grey solid. Many polytypes descr. Cation exchange capacity 0.1–0.4 eq kg^{-1}.

Steinfink, H., *Acta Crystallogr.*, 1958, **11**, 191, 195 (*cryst struct*)
Brown, B.E. *et al, Am. Mineral.*, 1962, **47**, 819 (*powder struct*)
Drits, V.A., *Acta Crystallogr., Sect. B*, 1969, **25**, 632 (*polytypes*)
Bailey, S.W., *Clays Clay Miner.*, 1988, **36**, 193 (*identification*)

$Al_2H_{10}O_{10}^{4\ominus}$ IC-000300
Aluminate ($Al_2(OH)_{10}^{4\ominus}$)
Di-μ-hydroxyoctahydroxydialuminate(4−)



M 224.0 (ion)
Di-Ba salt: Aluminium barium hydroxide ($Al_2Ba_2(OH)_{10}$). *Barium aluminate* ($Ba_2(Al_2(OH)_{10})$)
Synth. from Al_2O_3, BaO in H_2O. White prisms (H_2O). AlO_6 octahedra share edges to give $[Al_2(OH)_{10}]^{4\ominus}$ ions which form a lattice with $Ba^{2\oplus}$. Similar compd. $Al_2Ba_3(OH)_{12}$ also descr.

Ahmed, A.H.M. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 2169; 1970, **26**, 867 (*synth, cryst struct, Ba salt*)
Louis, R. *et al, Bull. Soc. Chim. Fr.*, 1969, 3471 (*synth, Ba salt*)

$Al_2H_{18}O_{10}^{4\oplus}$ IC-000302
Octaaquadi-μ-hydroxydialuminium(4+)
[46130-83-0]

$[(H_2O)_4Al(\mu\text{-}OH)_2Al(OH_2)_4]^{4\oplus}$

M 232.0 (ion)
Bis(sulfate) dihydrate: Aluminium hydroxide sulfate pentahydrate. Basic aluminium sulfate
$Al_2H_{22}O_{20}S_2$ M 460.2
Synth. from Al + H_2SO_4. Colourless cryst. (H_2O). Cations contain pairs of AlO_6 octahedra with shared edge, linked by H-bonds to anions and H_2O. Corresp. selenate is similar.

[36423-37-7]

Bassett, H. *et al, J. Chem. Soc.*, 1949, 2239 (*phase diagram, cryst struct, synth, sulfate*)
Johansson, G., *Acta Chem. Scand.*, 1962, **16**, 403 (*sulfate, synth, cryst struct, rel compd*)
Akitt, J.W. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 604 (*Al-27 nmr*)
Turner, R.C., *Can. J. Chem.*, 1975, **53**, 2811 (*thermodyn data*)

$Al_2H_{18}O_{22}P_4$ IC-000303
Aluminium phosphate ($Al_2H_6(PO_4)_4$)
Aluminium hydrogen phosphate $Al_2O_3{\cdot}2P_2O_5{\cdot}9H_2O$

$Al_2[H_{1+2z}PO_4]_3(H_2O)_6[H_{3-3z}PO_4]$

M 547.9
Structure cont. PO_4 tetrahedra and aggregates of two AlO_6 octahedra linked by corners to two PO_4 tetrahedra. Synth. by slow cryst. of a soln. of $Al^{3\oplus}$ in 85% H_3PO_4 ($Al:PO_4$ 1:3). Colourless trigonal pyramids (H_2O).

Kneip, R. *et al, Z. Naturforsch., B*, 1979, **34**, 750 (*synth, cryst struct*)

Al_2HgS_4 IC-000304
Aluminium mercury sulfide (Al_2HgS_4)
[12359-81-8]

$HgAl_2S_4$

M 382.8
Low pressure phase has tetragonal $CdGa_2S_4$ struct.: 3-coord. S are ccp and Al, Hg are tetrahedral. High pressure spinel phase also known. Synth. from HgS and Al_2S_3. Black solid. Band gap 2.54 eV.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)
Range, K.J. *et al, Z. Naturforsch., B*, 1968, **23**, 1009 (*high press form*)

Al_2HgSe_4 IC-000305
Aluminium mercury selenide (Al_2HgSe_4)

$HgAl_2Se_4$

M 570.3
Low pressure phase has tetragonal $CdGa_2S_4$ struct.: 3-coord. S are ccp and Al, Hg are tetrahedral. High pressure spinel phase also known. Synth. from Al_2Se_3 + HgSe. Black solid.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)
Range, K.J. *et al, Z. Naturforsch., B*, 1968, **23**, 1009 (*cryst struct*)

Al_2HgTe_4 IC-000306
Aluminium mercury telluride (Al_2HgTe_4)

$HgAl_2Te_4$

M 764.9
Statistical distribution of Hg and Al over metal sites in tetragonally distorted zinc blende lattice. Black solid.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)

$Al_2I_7^\ominus$ IC-000307
Heptaiododialuminate(1−)
μ-Iodohexaiododialuminate(1−)
[12588-50-0]

$[I_3AlIAlI_3]^\ominus$

M 942.2 (ion)
Li salt: Aluminium lithium iodide (Al_2LiI_7)
From $LiAlH_4$ + HI in C_6H_6. Colourless moisture-sensitive cryst. Insol. alkanes, dioxan, CS_2, spar. sol. Py; sol. Et_2O, DMSO, MeCN. Mp 220°. Monomeric in C_6H_6.
Na salt: Aluminium sodium iodide (Al_2NaI_7)
Al_2I_7Na M 965.2

Colourless moisture-sensitive solid. $NaAl_2I_{10}$ also descr. *Cs salt:* [12377-06-9]. *Aluminium caesium iodide* (Al_2CsI_7)

Al_2CsI_7 M 1075.2
Colourless moisture-sensitive solid. Mp 205°.

Evans, G.G. *et al*, *J. Inorg. Nucl. Chem.*, 1957, **4**, 48 (*cond*)
Klanberg, F. *et al*, *Chem. Ber.*, 1961, **94**, 781 (*synth*)
Boef, G. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **353**, 93 (*phase diagram*)
Mikheeva, V.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1012 (*phase diagram*)
Arkhipov, S.M. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 419 (*phase diagram, ternary syst*)
Begun, G.M. *et al*, *Inorg. Chem.*, 1971, **10**, 886 (*raman*)
Mikheeva, V.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1975, **24**, 1194 (*powder struct*)
Manteghetti, A. *et al*, *Spectrochim. Acta, Part A*, 1982, **38**, 141 (*raman, ir*)

Al_2Li_3 IC-000308

Aluminium compd. with lithium (2:3), 9CI

Aluminium lithium (Al_2Li_3). *Lithium aluminium* (Li_3Al_2)

[51846-18-5]

Al_2Li_3

M 74.7
Struct. has layers Al_n of puckered 6-membered rings with Li's between. Synth. from elements at 600°. Hard brittle grey moisture-sensitive solid alloy. Mp 520°.

Tebbe, K.-F. *et al*, *Z. Naturforsch., B*, 1973, **28**, 600 (*phase diagram, synth, cryst struct*)
Selman, J.R. *et al*, *J. Electrochem. Soc.*, 1977, **124**, 1160 (*thermodyn*)

Al_2MgO_4 IC-000309

Aluminium magnesium oxide (Al_2MgO_4)

Magnesium aluminate. Magnesium dialuminium oxide

[12068-51-8]

$MgAl_2O_4$

M 142.2
Structural prototype. Prepd. either from MgO + Al_2O_3 in PbF_2 at 1160-1290° or by reaction of $MgCl_2$ and Al(OAc)$_3$ at 1400°. Adsorbent for removing surfactants from H_2O. Catalyst. Support for transition metal and lanthanide phosphors. Colourless cubic cryst. Mp 1775°, Mp 2030-2060°. ΔH_f° −2299 (−2306) kJ mol^{-1}; ΔG_f° −2177 kJ mol^{-1}; S° 89 (81) J K^{-1} mol^{-1}. n_D 1.727. Forms mixed cryst. with $LiAlO_2$ and β-quartz. Not attacked by common acids or NaOH. Sl. etched by HF.

Mineral-form [1302-67-6]

Spinel

Parent of a large group of cubic mixed oxides of formula AB_2O_4. Common metamorphic mineral. May be various shades of red, blue, green, brown or black.

Swanson, H.E. *et al*, *Natl. Bur. Std. Circ. (U.S.)*, 1953, **2**, 38 (*cryst struct*)
Prasad, S. *et al*, *J. Indian Chem. Soc.*, 1956, **33**, 261; *CA*, **50**, 15035i (*synth*)
Hafner, S., *Z. Kristallogr.*, 1961, **115**, 331 (*ir*)
Beal, G.H. *et al*, *J. Am. Ceram. Soc.*, 1967, **50**, 181 (*phase diagram*)
Tarte, P. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2127 (*ir*)
Wood, J.D.C. *et al*, *J. Crystal Growth*, 1968, **3,4**, 489 (*synth*)
Padilla, F.C. *et al*, *J. Electrochem. Soc.*, 1968, **115**, 642 (*use*)
Navrotsky, A. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 479 (*synth, thermodyn*)
Rosenberg, M. *et al*, *J. Appl. Phys.*, 1970, **41**, 1114 (*Al-27 nmr*)
Geskovich, C. *et al*, *J. Phys. Chem. Solids*, 1970, **31**, 639 (*props*)
Messier, D.R. *et al*, *Am. Ceram. Soc. Bull.*, 1972, **51**, 692 (*synth*)
Bullens, M. *et al*, *J. Am. Ceram. Soc.*, 1978, **61**, 81 (*esca*)
Haycock, D.E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1785 (*pe*)
Bates, J.L. *et al*, *J. Am. Ceram. Soc.*, 1981, **64**, C138 (*elect cond*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 149 (*thermochem data*)
Müller, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1277 (*Al-27 nmr*)

$MgAl_2Te_4$ IC-000310

Aluminium magnesium telluride ($MgAl_2Te_4$)

[56831-86-8]

$MgAl_2Te_4$

M 588.6
Distorted defect zinc blende struct. Synth. from elements at 650-1000°. Red v. air- and moisture-sensitive cryst.

Dotzel, P. *et al*, *Z. Naturforsch., B*, 1975, **30**, 179 (*synth, cryst struct*)

$Al_2Mg_2O_{11}Si_3$ IC-000311

Simaldrate, INN

Tris[metasilicato(2−)]dioxodimagnesium(1:2) aluminate(4−), 9CI. Silodrate, USAN. Aluminosilicic acid magnesium salt. MP 1051

[12408-47-8]

M 362.8
Antacid. Fine white powder.

U.K. Pat., 1 153 513, (1969); *CA*, **71**, 126618s (*synth*)
Schnekenburger, J., *Arzneim.-Forsch.*, 1974, **24**, 142 (*pharmacol*)

$Al_2Mg_3O_{12}Si_3$ IC-000312

Pyrope

[1302-68-7]

$Al_2Mg_3[SiO_4]_3$

M 403.1
Magnesium aluminium silicate garnet. Can have Mg replaced by $Fe^{2\oplus}$ toward Almandine and by Mn toward Spessartine and Al replaced by $Cr^{3\oplus}$ toward Knorringite. Mineral which occurs in peridotites and associated serpentinites. A high-pressure phase in the system $MgO/Al_2O_3/SiO_2/H_2O$. Gemstone and abrasive. Cubic light pink or red cryst. May also be blue/green or violet.

Schreyer, W. *et al*, *Am. J. Sci., Part A*, 1969, **267**, 407 (*synth*)
Hazen, R.M. *et al*, *Am. Mineral.*, 1978, **63**, 297 (*cryst struct*)
Schmetzer, K. *et al*, *Neues Jahrb. Mineral., Abh.*, 1979, **136**, 146 (*ir*)
Ohashi, H. *et al*, *Ganseki Kobutsu Kosho Gakkaishi*, 1981, **76**, 58 (*cryst struct*)
Deer, W.A. *et al*, *Rock Forming Minerals*, 2nd Ed., Longman, London, 1982, **1A**, 498 (*rev*)
Viuko, V.I. *et al*, *Mineral. Zh.*, 1983, **5**, 42 (*ir*)
Aines, R.D. *et al*, *Am. Mineral.*, 1984, **69**, 1116 (*ir*)
Duroc-Danner, J.M., *J. Gemmol.*, 1984, **19**, 311.

$Al_2Mg_5Se_8$ IC-000313

Aluminium magnesium selenide ($Al_2Mg_5Se_8$)

Magnesium tetraselenoxoaluminate (5:2), 10CI

[65888-56-4]

$Al_2Mg_5Se_8$

M 807.1

Struct. is related to olivine and Li_3PO_4 with Mg in octahedral coordination and tetrahedral Al. Synth. from elements at 1000°. Almost colourless translucent moisture-sensitive cryst.

Dotzel, K.-P. *et al*, *Z. Naturforsch., B*, 1977, **32**, 1488 (*synth, cryst struct*)

Al_2MnO_4 IC-000314

Aluminium manganese oxide (Al_2MnO_4), 11CI

[12068-52-9]

$MnAl_2O_4$

M 172.8
Cubic spinel struct. Synth. from MnO and Al_2O_3 at 1000° in absence of O_2. Colourless solid. Antiferromagnetic below $T_N \simeq 18.5$K.

Greenwald, S. *et al*, *J. Chem. Phys.*, 1954, **22**, 1597 (*synth, magnetism*)
Scott, E.J., *J. Chem. Phys.*, 1955, **23**, 2459 (*synth*)
Roth, W.L., *J. Phys. (Paris)*, 1964, **25**, 507 (*struct, magnetic struct*)
Friedman, E.A. *et al*, *Phys. Rev.*, 1966, **147**, 457 (*magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1975, C3, 2 (*rev, bibl*)

Al_2MnS_4 IC-000315

Aluminium manganese(*II*) sulfide (Al_2MnS_4), 11CI

[12522-87-1]

$MnAl_2S_4$

M 237.1
Prepd. from elements at 600-1000°. Golden yellow cryst.

I-form

Stable-form

Rhombohedral modification.

II-form

Spinel struct. stable at high pressures.

Houdard, M., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1907, **144**, 801 (*synth*)
Flahaut, J., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1951, **233**, 1279 (*synth*)
Flahaut, J., *Ann. Chim. (Paris)*, 1952, **7**, 632 (*synth*)
Lappe, F. *et al*, *Z. Kristallogr.*, 1962, **117**, 146 (*struct*)
Donohue, P.C., *J. Solid State Chem.*, 1970, **2**, 6 (*struct, magnetism*)
Yokota, M. *et al*, *J. Solid State Chem.*, 1971, **3**, 520 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1976, **C6**, 52 (*rev, bibl*)

$Al_2Mo_3O_{12}$ IC-000316

Aluminium molybdenum oxide ($Al_2Mo_3O_{12}$)

Aluminium molybdate ($Al_2(MoO_4)_3$)

[15123-80-5]

$Al_2(MoO_4)_3$

M 533.7
Isostructural with $Fe_2(MoO_4)_3$ and $Cr_2(MoO_4)_3$. Monoclinic, interatomic distances, O—Al 188, O—Mo 169.8-181.2 pm. Prepd. by precipitation from Al salts and molybdic acid and subsequent calcining or from Al_2O_3 and MoO_3 in a Pt crucible at 700°. Commercially available. White powder. Mp 940-965°.

Plyasova, L.M. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1967, **3**, 906; *CA*, **69**, 55156k (*synth*)
Harrison, W.T.A. *et al*, *J. Solid State Chem.*, 1988, **76**, 328 (*cryst struct, nd*)

Al_2NNb_3 IC-000317

Aluminium niobium nitride (Al_2Nb_3N), 11CI

Triniobium dialuminium nitride

[12004-34-1]

Al_2Nb_3N

M 346.6
β-Manganese struct. The only stable ternary phase in the Al-Nb-N_2 system. It is stable in the range 1000-1500° and melts congruently. Synth. by heating a Nb/Al alloy with AlN.

Jeitschko, W. *et al*, *Monatsh. Chem.*, 1964, **95**, 1212 (*synth, cryst struct*)
Schuster, J.C. *et al*, *Z. Metallk.*, 1985, **76**, 728 (*synth, cryst struct, phase diagram*)

$Al_2Na_2O_{48}Si_{22}$ IC-000318

Zeolite Theta-1

$Na_n[Al_nSi_{24-n}O_{48}] \sim 4H_2O$, $n < 2$

M 1485.7
Limiting formula given. Zeolite struct. TON with 1D - channels 440 × 550 pm across and $(AlSi—O)_{10}$ rings. Synth. from $Na_2O—Al_2O_3—SiO_2—H_2O—H_2N(CH_2)_nNH_2$ gels at 180°. Has applications involving shape-selective adsorption. Colourless microcryst rods (aq. melt). ZSM-22, ZSM-23 (Zeolite struct MTT), Zeolite Nu-10 are similar.

Barri, S.A.I. *et al*, *Nature (London)*, 1984, **312**, 533 (*cryst struct, props*)
Araya, A. *et al*, *Zeolites*, 1984, **4**, 280 (*synth*)
Highcock, R.M. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 1391 (*cryst struct*)
Kokotailo, G.T. *et al*, *Zeolites*, 1985, **5**, 349 (*cryst struct*)
Rohrman, A.C. *et al*, *Zeolites*, 1985, **5**, 352 (*cryst struct*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 106, 134 (*struct*)
Harrison, I.D. *et al*, *Zeolites*, 1987, **7**, 28 (*adsorption*)
Marler, B., *Zeolites*, 1987, **7**, 393 (*synth, cryst struct*)
Thomas, J.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 434 (*em*)

Al_2NiO_4 IC-000319

Aluminium nickel(*II*) oxide (Al_2NiO_4)

[12004-35-2]

$NiAl_2O_4$

M 176.6
An inverse spinel. Synth. from NiO and Al_2O_3 at 1300°. Methanation and dehydrogenation catalyst.

Tarte, P., *Spectrochim. Acta, Part A*, 1967, **23**, 2127 (*ir*)
Navrotsky, A. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 479 (*synth, props*)
Reed, J.S., *J. Am. Ceram. Soc.*, 1975, **56**, 525 (*electronic props*)

Al_2O IC-000320

Aluminium(*I*) oxide (Al_2O)

[12004-36-3]

AlOAl (C_{2v})

M 69.9
Detected in gas phase, in Ar or Kr matrices, or possibly at Al/Al_2O_3 interfaces; Al—O 172 pm, AlOAl 144°. ΔH_f −138 kJ mol^{-1}.

Drowart, J. *et al*, *J. Chem. Phys.*, 1959, **32**, 1366 (*synth, thermodyn props*)

Linevsky, M.J. *et al, J. Chem. Phys.*, 1964, **41**, 542 (*ir*)
Burns, R.P. *et al, J. Chem. Phys.*, 1966, **44**, 3307 (*ms, thermodyn props*)
Makowiecki, D.M. *et al, J. Phys. Chem.*, 1971, **75**, 1963 (*ir*)
Farber, M. *et al, J. Chem. Soc., Faraday Trans. 1*, 1972, **68**, 249 (*ms, thermodyn, props*)
Marino, C.P. *et al, J. Phys. Chem.*, 1973, **77**, 2929 (*ir*)
Ivanov, A.A. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1973, **14**, 854 (*ed*)
Lynch, D.A. *et al, J. Phys. Chem.*, 1974, **78**, 236 (*ir*)

IC-000321

Al_2O_3

Aluminium oxide (Al_2O_3)

Alumina. Alundum. Aloxite

[1344-28-1]

Al_2O_3

M 101.9

Commercially available. White solid. Sol. hot NaOH.

▷ BD1200000.

Hydrate: [12043-15-1]. ***Akdalaite***
Mineral from Kazakhstan, USSR. White translucent cryst.

α-form [1302-74-5]
Corundum. Emery
High temp. modification, indefinitely metastable at r.t. Structural prototype comprising hcp oxide with Al in O_4 holes; solid solns. with small amounts of M_2O_3 give rise to various gem varieties. Mineral of haematite group of widespread occurrence or may by synth. from γ-form or any hydrous oxide ⩽450°. Gem quality corundum known as White sapphire. Abrasive. Transparent cryst; v. hard, resistant to attack by acids. Mp 2323°. ΔH_f° *ca.* −1682 kJ mol^{-1}; S° 50.9 JK^{-1} mol^{-1}; E_g > 5 eV.

▷ GN0231000.

Mixed oxide with Cr_2O_3: [12174-49-1]. ***Ruby***
Occurs naturally or may be synth. from NH_4 (Al,Cr) alums at 1450°. Used in lasers and masers; gem. Brilliant red cryst. Red colour imparted by 1-4% Cr_2O_3.

Mixed oxide with Fe, Ti: [1317-82-4]. ***Sapphire. Blue sapphire***
Gem. Transparent blue cryst.

β-form
Not a simple polymorph. Always contains alkali metal cations: see *Aluminium sodium oxide* ($Al_{11}NaO_{17}$), IC-000395 and *β″ alumina* Al_2NaO_4.

γ-form
Defect spinel struct. Li required. Stabilised by AlN. White solid; readily takes up H_2O and dissolves in acids. Forms on oxidised Al surfaces.

Surface film-form
Has defect NaCl struct. Protects Al surfaces from oxidation.

[12252-63-0, 12522-88-2]

Brown, J.F. *et al, J. Chem. Soc.*, 1953, **84** (*synth*)
Schneider, A. *et al, Z. Anorg. Allg. Chem.*, 1954, **277**, 41.
Scholze, H., *Z. Anorg. Allg. Chem.*, 1956, **284**, 272 (*related compds, powder struct*)
Kauer, E. *et al, Z. Naturforsch., A*, 1958, **13**, 531 (*optical props*)
Jan, J.P., *Helv. Phys. Acta*, 1960, **33**, 123 (*ruby, powder struct*)
Long, G. *et al, J. Am. Ceram. Soc.*, 1961, **44**, 255 (*phase diagram*)
Litz, A., *Phys. Rev.*, 1961, **123**, 501 (*ruby, uv-vis*)
McClure, D.S., *J. Chem. Phys.*, 1962, **36**, 2757 (*ruby, uv-vis*)
Newnham, R.E. *et al, Z. Kristallogr.*, 1962, **117**, 235 (*cryst struct, α-form*)
Moss, S.C. *et al, Z. Kristallogr.*, 1964, **120**, 359 (*ruby, cryst struct*)
Burns, R.P. *et al, J. Chem. Phys.*, 1966, **44**, 3307 (*ms, thermodyn props*)
Tarte, P. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 2127 (*ir*)

Diggle, J.W., *Chem. Rev.*, 1969, **69**, 365 (*rev, surface films*)
Parker, H.S. *et al, J. Am. Ceram. Soc.*, 1970, **53**, 583 (*cryst growth*)
Farber, M. *et al, J. Chem. Soc., Faraday Trans. 1*, 1972, **68**, 249 (*ms, thermodyn*)
Sato, T., *Z. Anorg. Allg. Chem.*, 1972, **391**, 167 (*synth, phase transforms*)
McGuire, G.E. *et al, Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Nicholls, C.J. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 901 (*xre*)
Nukui, A. *et al, J. Am. Ceram. Soc.*, 1976, **59**, 534 (*props*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **1**, 33; **2**, 218; **5**, 240 (*rev*)
Ishizawa, N. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 228 (*cryst struct, α-form*)
Müller, D. *et al, Chem. Phys. Lett.*, 1981, **79**, 59 (*Al-27 nmr*)
Alford, N.Mc.N., *Nature (London)*, 1987, **330**, 51 (*use*)
Burkin, A.R., *Prod. Alum. and Alumina, 1987*, Wiley, 1987.
Zecchina, A. *et al, Inorg. Chem.*, 1988, **27**, 102 (*synth, use*)
Hart, L.D. *et al, Aluminium Chems. Sci. and Tech. Handbook*, Am. Ceram. Soc., 1990.

IC-000322

Al_2O_4Pb

Aluminium lead oxide (Al_2PbO_4)

Lead aluminate ($PbAl_2O_4$)

[1345-29-5]

$PbAl_2O_4$

M 325.1

Tridymite-like struct. with Pb as interstices. Synth. from PbO + Al_2O_3 at 900-1100°. Cryst. Similar compds. $Pb_2Al_2O_5$, $PbAl_{12}O_{19}$ descr.

Glasser, F.P. *et al, J. Am. Ceram. Soc.*, 1963, **46**, 377 (*synth, cryst struct*)
Harari, A. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **264**, 84 (*cryst struct, phase diagram*)
Ploetz, K.B. *et al, Z. Anorg. Allg. Chem.*, 1982, **488**, 38 (*synth, cryst struct*)

IC-000323

Al_2O_4Sr

Aluminium strontium oxide (Al_2SrO_4)

[12004-37-4]

$SrAl_2O_4$

M 205.5

Tridymite (SiO_2) struct. with Sr in the interstices. Synth. from Al_2O_3 and $SrCO_3$ at 1200°. Support for lanthanide phosphors. Colourless cryst. (melt). Phase transition occurs at 650°. Related compd. Al_4SrO_7 also descr.

Lagerqvist, K. *et al, Z. Anorg. Allg. Chem.*, 1937, **234**, 1 (*synth*)
Glasser, F.P. *et al, J. Am. Ceram. Soc.*, 1963, **46**, 377 (*synth, cryst struct*)
Palilla, F.C. *et al, J. Electrochem. Soc.*, 1968, **115**, 642 (*use*)
Ito, S. *et al, Z. Phys. Chem. (Munich)*, 1977, **105**, 173; **107**, 50 (*phase transition, solid solns*)
Schulze, A.-R. *et al, Z. Anorg. Allg. Chem.*, 1981, **475**, 205 (*cryst struct*)
Machida, K.-I. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 889 (*cryst struct, Al_4SrO_7*)

Al_2O_4Zn IC-000324

Aluminium zinc oxide (Al_2ZnO_4)

Zinc aluminate ($ZnAl_2O_4$)

[12068-53-0]

$ZnAl_2O_4$

M 183.3

Spinel-type struct. Pigment; abrasive; used in glass ceramics; in anti-corrosion coatings; moisture sensors; catalyst for oxidations of organics, aromatisation, dehydrogenation; catalyst in hydrogenation cracking and in reforming hydrocarbons. Used in screen printable dielectric compds. for printed circuits. Cryst.

Clark, G.L. *et al, Am. J. Sci.*, 1931, **22**, 539 (*lattice dimensions*)
Swanson, H.E. *et al, Natl. Bur. Std. Circ. (U.S.)*, 1953, **II**, 539 (*powder struct*)
Vermaas, F.H.S. *et al, Beitr. Mineral. Petrogr.*, 1959, **6**, 219 (*synth, struct*)
Lutz, H.D. *et al, Spectrochim. Acta, Part A*, 1971, **27**, 357 (*ir*)
Koningstein, J.A. *et al, J. Chem. Phys.*, 1972, **56**, 354 (*raman*)
Ogilvie, J.L. *et al, Chem. Technol.*, 1973, 567 (*esca*)
Hikuhara, Y. *et al, Yogyo Kyokaishi*, 1983, **91**, 281 (*synth*)
Yamakawa, A. *et al, J. Mater. Sci.*, 1989, **24**, 1491 (*cryst growth*)

Al_2O_5Si IC-000325

Andalusite

[12183-80-1]

Al_2SiO_5

M 162.0

Struct. comprises chains of distorted AlO_6 octahedra sharing edges, SiO_4 tetrahedra and pairs of edge-sharing AlO_5 trigonal bipyramids. Occurs chiefly in slates and argillaceous schists as a contact mineral. Found in USA, Canada, Brazil, Spain, USSR, Korea, Australia and elsewhere. Refractory in steel industry. Cryst. various colours usually pink, redish brown, rose red. See also Kyanite, IC-000326.

Burnham, C.W. *et al, Z. Kristallogr.*, 1961, **115**, 269 (*cryst struct*)
Holm, J.L. *et al, Am. Mineral.*, 1966, **51**, 1608 (*thermodyn props*)
Hafner, S.S. *et al, J. Chem. Phys.*, 1970, **52**, 6037 (*Al-27 nqr*)
Winter, J.K. *et al, Am. Mineral.*, 1979, **64**, 573 (*cryst struct*)
Smith, K.A. *et al, Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)
Mägi, M. *et al, J. Phys. Chem.*, 1984, **88**, 1518.
Lippmaa, E. *et al, J. Am. Chem. Soc.*, 1986, **108**, 1730 (*Al-27 nmr*)

Al_2O_5Si IC-000326

Kyanite

Cyanite. Diothene. Aluminium oxide silicate ($Al_2O(SiO_4)$)

[1302-76-7]

Al_2SiO_5

M 162.0

Orthosilicate struct. with ccp oxygen, SiO_4 tetrahedra, octahedrally coord. Al. Mineral found in USA, India, Kenya, Romania, Australia and elsewhere. Usually blue long bladed cryst. colour often varies in single cryst.; also white, grey, green, yellow, pink or nearly black. See also Andalusite, IC-000325.

▷ BD1450000.

Holm, J.L. *et al, Am. Mineral.*, 1966, **51**, 1608 (*thermodyn props*)
Winter, J.K. *et al, Am. Mineral.*, 1979, **64**, 573 (*cryst struct*)
Smith, K.A. *et al, Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)
Mägi, M. *et al, J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)
Javes, N. *et al, J. Am. Chem. Soc.*, 1985, **107**, 6769 (*Si-29 nmr*)
Lippmaa, E. *et al, J. Am. Chem. Soc.*, 1986, **108**, 1730 (*Al-27 nmr*)

Al_2O_5Si IC-000327

Sillimanite

[12141-45-6]

Al_2SiO_5

M 162.0

Struct. contains double chains of SiO_4 and AlO_4 tetrahedra sharing corners and octahedrally coordinate Al between. Isomorphous replacement Al by Fe. Obt. from fused oxides. Mineral in sands and metamorphic rocks. Ceramic component, refractory, molding sand, cracking and isomerisation catalyst. White solid. Mp 1816°. ΔH_f° −2584.4 kJ mol^{-1}. Thermal cond. 1.59 W K^{-1} m^{-1}. Thermal exp. 5.4 × 10^{-6}.

Agrell, S.O. *et al, J. Am. Ceram. Soc.*, 1960, **43**, 69 (*cryst struct, optical data*)
Holm, J.L., *Am. Mineral.*, 1966, **51**, 1608 (*thermodyn*)
Raymond, M. *et al, J. Chem. Phys.*, 1970, **53**, 4110 (*Al-27 nqr*)
Howald, R.A. *et al, J. Phys. Chem.*, 1978, **82**, 2199 (*thermodyn*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 247; **24**, 865 (*rev*)
Winter, J.K. *et al, Am. Mineral.*, 1979, **64**, 573 (*cryst struct*)
Smith, K.A. *et al, Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)
Mägi, M. *et al, J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

$Al_2O_{12}S_3$ IC-000328

Aluminium sulfate ($Al_2(SO_4)_3$)

$Al_2(SO_4)_3$

M 342.1

Obt. from hydrates at 325°. Used in water purif. (flocculant). Size for paper. Commercially available. White solid. Forms complex series of hydrates. Dec. at 450° to amorphous Al_2O_3 with high surface area. $\Delta H_{f\,298}^\circ$ −3435 kJ mol^{-1}. $Al(HSO_4)_3$ also known.

17 Hydrate: ***Alunogen***
Mineral, occurs mainly as an efflorescence or cavity filling in slates and shales. Colourless cryst.

18 Hydrate: [7784-31-8].
Obt. from bauxite or clay + H_2SO_4. Colourless hygroscopic cryst. (H_2O). Exact amount of H_2O uncertain. Gives anhydrous salt during 24h at 380°.

Sodium alum: see *Aluminium sodium sulfate* ($AlNa(SO_4)_2$), *IC-000223*

Potassium alum: see *Aluminium potassium sulfate* ($AlK(SO_4)_2$), *IC-000203*

Caesium alum: see *Aluminium caesium sulfate dodecahydrate, IC-000150*

Young, F.E., *J. Am. Chem. Soc.*, 1945, **67**, 257 (*synth, thermodyn data*)
Bassett, H. *et al, J. Chem. Soc.*, 1949, 2239 (*synth, phase diagram, powder struct, hydrates, props*)
Kellogg, H.H., *Trans. Metall. Soc. AIME*, 1964, **230**, 1622 (*thermodyn data*)
Vandorpe, B. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1973, **277**, 1121 (*related compd*)
Akitt, J.W. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1226 (*Al-27 nmr*)
Knutsen, G.F. *et al, J. Electrochem. Soc.*, 1978, **125**, 327 (*dec*)

$Al_2O_{12}Se_3$ IC-000329

Aluminium selenate ($Al_2(SeO_4)_3$)

$Al_2(SeO_4)_3$

M 482.8

Synth. from $Al(OH)_3$ and H_2SeO_4. Several hydrates and a basic salt similar to Octaaquadi-μ-hydroxydialuminium(4+), IC-000302 also descr.

Hexadecahydrate: Colourless hexagonal plates (H_2O). Sol. H_2O; spar. sol. EtOH.

Bassett, H., *J. Chem. Soc.*, 1950, 1191 (*synth, phase diagram*)
Johansson, G., *Acta Chem. Scand.*, 1962, **16**, 403 (*cryst struct, basic salt*)
Selivanova, N.M., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1963, **8**, 857 (*synth, tga*)

Al_2PbS_4 IC-000330

Aluminium lead sulfide (Al_2PbS_4)

Lead thioaluminate

[11078-39-0]

Al_2PbS_4

M 389.4

Prepd. by heating PbS, Al and S mixts. Light-grey cryst. Easily hydrol. Mp 860°

Monselise, G.G. *et al*, *Gazz. Chim. Ital.*, 1937, **67**, 511 (*synth*)
Flahaut, J., *Ann. Chim. (Paris)*, 1952, **7**, 632 (*synth*)
Eholie, R. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 747 (*synth, struct*)

Al_2PbSe_4 IC-000331

Aluminium lead selenide (Al_2PbSe_4)

[11078-40-3]

Al_2PbSe_4

M 577.0

Prepd. by heating PbS, Al and Se mixts. Cryst.

Eholie, R. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 747 (*synth*)
Klee, W. *et al*, *Mater. Res. Bull.*, 1980, **15**, 1033 (*cryst struct*)

Al_2S_3 IC-000332

Aluminium sulfide (Al_2S_3)

[1302-81-4]

Al_2S_3

M 150.1

Commercially available. Moisture-sensitive white cryst. (melt). Mp 1100° (1240°). E_g 4.1 eV (300K); ΔH_f° −726 kJ mol^{-1}

Monoclinic-form

α-form

Distorted wurtzite struct. From the elements at 700-1000°. Moisture-sensitive colourless cryst.

Cubic-form

Cation deficient spinel struct. which is stabilised at ambient pressure by inclusion of ~2% As. Formed from elements at 400° and 4 × 10^4 atm. Colourless moisture-sensitive cryst.

Tetragonal-form

Has spinel struct. similar to β-In_2S_3. Obt. from elements at 2-65 × 10^3 atm. at 1000°. Yellow orange v. moisture-sensitive cryst. Semiconductor, E_g 0.3 eV; conductivity 10^{-7} Ω^{-1} m^{-1} at 25°.

Hexagonal β-form

Obt. from elements in presence of Al_4C_3 at 1000-1100°. Has disordered wurtzite struct.

Hexagonal γ-form

Has α-Al_2O_3 struct. Stable between 1000-1100°.

Kauer, E. *et al*, *Z. Naturforsch., A*, 1958, **13**, 531 (*optical props*)
Schäfer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **325**, 77 (*cryst struct, cubic form*)
Donohue, P.C., *J. Solid State Chem.*, 1970, **2**, 6 (*cryst struct, tetragonal form*)
Gromakov, S.D. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1972, **46**, 91 (*props*)
McGuire, G.E. *et al*, *Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Range, K.-J. *et al*, *Z. Naturforsch., B*, 1973, **28**, 353 (*synth, cryst struct, cubic form*)
Foerland, T. *et al*, *Acta Chem. Scand., Ser. A*, 1974, **28**, 226 (*phase diagram*)
Bonsall, S.B. *et al*, *J. Solid State Chem.*, 1978, **25**, 379 (*phase diagram*)
Hellstrom, E.E. *et al*, *Mater. Res. Bull.*, 1979, **14**, 127 (*synth, α-form*)
Berg, R.W. *et al*, *Inorg. Chem.*, 1980, **19**, 2688 (*raman*)
Haeuseler, H. *et al*, *Z. Naturforsch., B*, 1981, **36**, 532 (*ir, raman*)

Al_2S_4Sr IC-000333

Aluminium strontium sulfide (Al_2SrS_4)

Strontium thioaluminate

[11078-41-4]

Al_2SrS_4

M 269.8

Prepd. by heating SrS, Al and S mixts. Cryst.

Eholie, R. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 747 (*synth, cryst struct*)

Al_2S_4Zn IC-000334

Aluminium zinc sulfide (Al_2ZnS_4)

[12271-58-8]

$ZnAl_2S_4$

M 247.6

α-form has cubic spinel struct., β-form hexagonal wurtzite superlattice and γ-form has rhombohedral defect $ZnIn_2S_4$ struct. Spinel form may be converted to wurtzite struct. >1000°. Synth. from ZnS, Al and S at 800°. Colourless cryst. Slow reaction with moist air → H_2S. Sr, Pb, Cr, Mn, Fe, Cd and Hg analogues also descr.

Flahaut, J., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1951, **233**, 1279 (*synth, rel compds*)
Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1952, **269**, 227.
Steigman, G.A. *et al*, *Acta Crystallogr.*, 1967, **23**, 142 (*cryst struct*)
Eholie, R. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 747 (*similar compds*)
Lutz, H.D. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 357 (*ir*)
Bonsall, S.B. *et al*, *J. Solid State Chem.*, 1978, **25**, 379 (*phase diagram*)
Berthold, H.J. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **475**, 45 (*cryst struct*)

Al_2Se IC-000335

Aluminium(*I*) selenide (Al_2Se)

Al_2Se

M 132.9

Not isol. pure. Synth. from Cu_2Se + Al. Grey-black solid with metallic sheen. Rapid dec. in air. $Bp_{0.01}$ 1200°.

Schneider, A. *et al*, *Z. Anorg. Allg. Chem.*, 1954, **277**, 49 (*synth*)

Al_2Se_3 IC-000336

Aluminium selenide (Al_2Se_3)

[1302-82-5]

Al_2Se_3

M 290.8

Dimorphic. Commercially available. E_g 3.1 eV.

Cubic-form

Cation deficient spinel struct. Synth. from elements at 6 x 10^4 atm. and 600°. Grey moisture-sensitive cryst.

Hexagonal-form

Cation deficient wurtzite struct. Synth. from elements at 1000°. Grey moisture-sensitive solid (melt). Mp 980°. ΔH_f° −543 kJ mol^{-1}.

Inorg. Synth., 1946, **2**, 183 (*synth*)
Klemm, W. *et al*, *Z. Anorg. Allg. Chem.*, 1948, **255**, 287 (*synth, phase diagram*)

Schneider, A. *et al*, *Z. Anorg. Allg. Chem.*, 1954, **277**, 49 (*cryst struct, hexagonal form*)
Kauer, E. *et al*, *Z. Naturforsch., A*, 1958, **13**, 531 (*optical props*)
Steigman, G.A. *et al*, *Acta Crystallogr.*, 1966, **20**, 617 (*cryst struct, hexagonal form*)
Gromakov, S.D. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1972, **46**, 91 (*props*)
Range, K.J. *et al*, *Z. Naturforsch., B*, 1973, **28**, 353 (*cryst struct, cubic form*)
Berg, R.W. *et al*, *Inorg. Chem.*, 1980, **19**, 2688 (*raman*)
Popović, S. *et al*, *J. Appl. Chem.*, 1980, **13**, 454 (*quaternary compds*)

Al_2Se_4Sr IC-000337

Aluminium strontium selenide (Al_2SrSe_4)

[11078-42-5]

$SrAl_2Se_4$

M 457.4

Possesses orthorhombic struct. related to TlSe with 4-coord. (T_d) Al and 8-coord. (square antiprismatic) Sr. Synth. from SrSe, Al and Se at 800°. Red moisture-sensitive cryst. Pb and Eu compds. also descr.

Eholie, R. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 747 (*synth, powder struct*)
Klee, W. *et al*, *Z. Naturforsch., B*, 1978, **33**, 829 (*cryst struct*)

Al_2Se_4Zn IC-000338

Aluminium zinc selenide (Al_2ZnSe_4)

[12359-83-0]

$ZnAl_2Se_4$

M 435.1

Low pressure phase has tetragonal $CdGa_2S_4$ struct.: 3-coord. S are ccp and Al, Zn are tetrahedral. High pressure spinel phase also known. Synth. from Al_2Se_3 + ZnSe. Black solid.

Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)
Range, K.J. *et al*, *Z. Naturforsch., B*, 1968, **23**, 1009 (*cryst struct*)

Al_2SrTe_4 IC-000339

Aluminium strontium telluride (Al_2SrTe_4)

[39297-20-6]

Al_2SrTe_4

M 651.9

Struct. resembles TlTe. Synth. from elements. Bright red prisms (melt).

Franke, E. *et al*, *Z. Naturforsch., B*, 1972, **27**, 1308.

Al_2Te_4Zn IC-000340

Aluminium zinc telluride (Al_2ZnTe_4)

[12421-34-0]

Al_2ZnTe_4

M 629.7

Al and Zn are statistically distributed over metal sites in tetragonally distorted zinc blende lattice. Black solid.

Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1955, **279**, 241 (*synth, powder struct*)

$Al_{2.3}H_2K_{0.9}Mg_{0.3}O_{12}Si_{3.4}$ IC-000341

Illite

[12173-60-3]

$K_{0.9}[Mg_{0.3}Al_{1.7}(Al_{0.8}Si_{3.4}O_{10})(OH)_2]$

M 394.0

Non-expanding clay mineral derived from Muscovite, IC-000351 by replacement of tetrahedral Al by Si and octahedral Al by Mg. Many variations in formulae. May be made hydrothermally from ammonium luminosilicate gels. Used in ceramics. Dull white solid; may also show various pale colours. Cation exchange capacity 0.2-0.4 eq kg^{-1}.

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1961, 971 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 190; **5**, 238; **6**, 200 (*rev, use*)
Kinsey, R.A. *et al*, *Am. Mineral.*, 1985, **70**, 537 (*Al-27, Si-29 nmr*)
Turner, G.L., *Am. Ceram. Soc. Bull.*, 1987, **66**, 6561 (*Al-27, Si-29 nmr*)

$Al_{2.5}Na_{2.5}O_{56}Si_{25.5}$ IC-000342

Zeolite ZSM-12

$Na_n[Al_nSi_{28-n}O_{56}].4H_2O$, $n < 2.5$

M 1737.0

Limiting formula listed. Zeolite struct. MTW with 1-D channels (550 × 590 pm across) and highly non-planar $(Al,Si—O)_{12}$ rings. Synth. from $Na_2O—SiO_2—Al_2O_3—H_2O$ mixt. + $MeEt_3NBr$. Catalyst in hydrocarbon conversions and separation of alkylbenzenes. White microcryst. solid (aq. melt). Zeolite beta similar: also found as mineral Tschernichite.

U.S. Pat., 33 08 069, (1967); *CA*, **67**, 26245.
LaPierre, R.B. *et al*, *Zeolites*, 1985, **5**, 346 (*cryst struct*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 108.
Ernst, S. *et al*, *Zeolites*, 1987, **7**, 458 (*synth*)
Davis, M.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 920.
Newsam, J.M. *et al*, *Proc. R. Soc. London, A*, 1988, **420**, 375 (*synth, cryst struct, powder struct, ed, em, zeolite beta*)
Weitkamp, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 1908 (*synth, zeolite beta*)
Smith, J.V. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 363 (*mineral*)
Corma, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 594 (*use*)

$Al_3Ca_2HO_{13}Si_3$ IC-000343

Clinozoisite, 9Cl

Klinozoisite

[1318-31-6]

$Ca_2Al_3[SiO_4][Si_2O_7]O(OH)$

M 454.3

Mineral of the epidote group. Dimorph of Zoisite. Occurs in regionally metamorphosed igneous and sedimentary rocks. Colourless, pale yellow, green, pink or grey monoclinic cryst.

Dollase, W.A., *Am. Mineral.*, 1968, **53**, 1882 (*cryst struct*)
Deer, W.A. *et al*, *Rock Forming Minerals*, 2nd Ed., Longman, London, 1986, **1B**, 44 (*rev*)

$Al_3ClNa_4O_{12}Si_3$ IC-000344

Sodalite

[1302-90-5]

$Na_6[Al_6Si_6O_{24}].2NaCl$

M 484.6

Zeolite struct. SOD. Parent of a group of cubic alumino silicates having general formula $(Na,Ca)_{4-8}Al_3Si_6(O,S)_{24}(SO_4,Cl,OH)$. 'Sodalite cages', comprising stacked 14-hedra (truncated octahedra) with apertures formed by $(Al,Si—O)_6$ rings, are commonly found in other zeolites (Zeolite A, etc.). Widely distributed mineral (incl. var. Hackmanite); hydrothermal synth. from aluminosilicate gels in presence of NaOH and $[Me_4N]OH$. White cryst. Mineral samples show various colours. n_D 1.483.

Chloride form:
$Al_6Cl_2Na_8O_{24}Si_6$ M 969.2
Mineral from Ontario, Canada. White solid.

Hydroxide form: Basic sodalite
$Al_6H_6Na_8O_{28}Si_6$ M 968.3
Made hydrothermally at 450° and 1.53×10^7 atm. Adsorbant for small molecules. Dodecahedral white cryst.

Sulfate form: Nosean. Noselite
$Al_6Na_8O_{28}SSi_6$ M 994.3

Ultramarine: [1317-97-1].
$Al_6Na_8O_{24}S_4Si_6$ M 1026.5
Contact metamorphic mineral Lapis lazuli (Lazurite) formulated as $(Na,Ca)_8(Al,Si)_{12}O_{24}[SO_4Cl_2(OH)_2]$. A related mineral is Hauyne or Hauynite which is also blue but formulated $(Na,Ca)_{4-8}Al_6Si_6(O,S)_{24}(SO_4,Cl)_{1-2}$. Synth. from kaolinite, S, NaOH + coke at 800°. Hydrothermal synth. at 410° and 5.5×10^5 atm. Pigment. Lapis lazuli used as gemstone. Blue cryst. Related green, violet and red substances cont. different S-cont. spp. also descr. Zeolite struct. SOD cont. $S_2^{\ominus}$ and $S_3^{\ominus}$ radical ions.

Me_4N form:
$C_4H_{12}AlNO_{12}Si_5$ M 433.5
From $(Me_4N)OH$, $Si(OMe)_4$, $Al(OPr^i)_3$ and H_2O at 100° then 180°. White cryst. (aq. melt).

Non-basic form:
$Al_3Na_3O_{12}Si_3$ M 426.1
White solid. Sodalite hydrates obt. from hydroxy form at 127°; anhydrous form by subsequent dehydration.

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1951, 195; 1952, 1561 (*synth*)
Barrer, R.M. *et al*, *Proc. R. Soc. London*, 1956, **236**, 227 (*ion exchange*)
Löns, J. *et al*, *Acta Crystallogr., Sect. B*, 1967, **23**, 434 (*cryst struct*)
Kroone, B., *Chem. Ind. (London)*, 1968, 287 (*reactions, ultramarine*)
Baerlocher, C. *et al*, *Helv. Chim. Acta*, 1969, **52**, 1853 (*cryst struct, Me_4N form*)
Holzer, W. *et al*, *J. Mol. Spectrosc.*, 1969, **32**, 13 (*raman, ultramarine*)
Hofmann, U. *et al*, *Z. Anorg. Allg. Chem.*, 1969, **367**, 119 (*synth, props, uv-vis, esr, ultramarine*)
Aiello, R. *et al*, *J. Chem. Soc. A*, 1970, 1470 (*synth*)
McLaughlan, S.D. *et al*, *J. Phys. Chem.*, 1970, **74**, 1359 (*synth, esr, ultramarine*)
Schwarz, K.-H. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **378**, 52 (*x-ray fluorescence, uv, ir, esr, ultramarine*)
Barrer, R.M. *et al*, *J. Phys. Chem. Solids*, 1971, **32**, 731 (*absorption*)
Henderson, C.M.B., *Spectrochim. Acta, Part A*, 1977, **33**, 283 (*ir*)
Clark, R.J.H. *et al*, *Inorg. Chem.*, 1978, **17**, 3169 (*raman, ultramarine*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4992 (*Si-29 nmr*)
Klinowski, J. *et al*, *J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Koch, E. *et al*, *Z. Kristallogr.*, 1981, **154**, 95 (*rev*)
Fyfe, C.A. *et al*, *J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Hassan, I. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 3 (*cryst struct, OH form*)
Hassan, I. *et al*, *Acta Crystallogr., Sect. B*, 1984, **40**, 6 (*cryst struct, Cl form, expansion*)
Depmeier, W., *Acta Crystallogr., Sect. B*, 1984, **40**, 185 (*rev*)
Felsche, J. *et al*, *Zeolites*, 1986, **6**, 367 (*cryst struct, non basic form*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 128.
Weller, M.T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 1103; 1991, 734 (*powder struct, Si-29 nmr, ir*)

IC-000345

$Al_3Cl_{12}Dy$

Hexa-μ-chlorotris(dichloroaluminium)dysprosium, 12Cl

Aluminium dysprosium chloride (Al_3DyCl_{12}). Dysprosium tris[tetrachloroaluminate(1−)]

[130725-68-7]

$DyAl_3Cl_{12}$

M 668.8
Similar compds. formed by other Ln. Antiprismatic struct. Involved in thermal vapour transport of $LnCl_3$ with $AlCl_3$; precursor in prepn. of pure $LnCl_3$. Colourless cryst. Dec. to $DyCl_3$ on heating.

Hake, D., *Z. Anorg. Allg. Chem.*, 1990, **586**, 99 (*synth, cryst struct*)

IC-000346

$Al_3Cl_{12}Ho$

Hexa-μ-chlorotris(dichloroaluminium)holmium, 10Cl

Holmium tetrachloroaluminate ($Ho(AlCl_4)_3$)

[123776-17-0]

$Ho[AlCl_4]_3$

M 671.3
$HoCl_8$ square antiprisms are linked via edges with $AlCl_4$ tetrahedra. Synth. from Ho_2O_3 + $AlCl_3$ by chem. vap. transport. Salmon-coloured air- and moisture-sensitive cryst. (from vap.). Similar Sm and Nd compds. descr. in gas phase.

Oøye, H.A. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 2229 (*Nd analogue*)
Papatheodorou, G.N. *et al*, *Inorg. Chem.*, 1979, **18**, 385 (*Sm analogue*)
Hake, D. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 1364 (*cryst struct*)

IC-000347

$Al_3Cl_{12}Nd$

Neodymiumhexa-μ-chlorohexachlorotrialuminium

Aluminium neodymium chloride (Al_3NdCl_{12}). Tris(tetrachloroaluminato)neodymium

[12408-49-0]

$NdAl_3Cl_{12}$

M 650.6
Formed in the vapour phase by vaporisation of solid $NdCl_3$ in the presence of Al_2Cl_6 gas.

[63643-30-1]

Oye, H.A. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 2229 (*formn, themodyn*)
Agafonov, I.L. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1980, **16**, 1088; *CA*, **93**, 105686b (*ms, thermodyn*)

IC-000348

$Al_3Cl_{12}Sm$

Samariumhexa-μ-chlorohexachlorotrialuminium

Aluminium samarium chloride (Al_3SmCl_{12}). Tris(tetrachloroaluminato)samarium

[68645-74-9]

$SmAl_3Cl_{12}$

M 656.7

Formed in the vapour phase by vaporisation of solid $SmCl_3$ in the presence of Al_2Cl_6 gas.

Papatheodorou, G.N. *et al*, *Inorg. Chem.*, 1979, **18**, 385 (*formn, thermodyn*)

IC-000349

$Al_3CsNa_2O_{24}Si_9$

Zeolite rho

$(Na,Cs)_{12}[Al_{12}O_{96}Si_{36}].n\ H_2O$

M 896.5
Zeolite struct. RHO. Member of faujasite group. Struct. comprises 2 non-intersecting 3-D interpenetrating channel structs. (360 pm diameter) of zeolite A type. A 26 hedron is linked by octagonal prisms through each of its 6 $(Al,Si—O)_8$ rings to an $(Al,Si—O)_8$ ring of 6 other 26 hedra. $Na^{\oplus}$, $Cs^{\oplus}$ may be replaced by $NH_4^{\oplus}$, $Ca^{2\oplus}$ etc. with considerable framework distortion. Synth. from aq. NaOH, CsOH, $Al(OH)_3$ and SiO_2 at 60-120°.

U.S. Pat., 3 720 753, (1973); *CA*, **79**, 33220 (*synth*)
Parise, J.B. *et al*, *J. Phys. Chem.*, 1984, **88**, 1635, 2303 (*nd*)
McCusker, L.B., *Zeolites*, 1984, **4**, 51 (*cryst struct NH_4-form*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 122.
Corbin, D.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 42 (*nd, Ca-form*)
Parise, J.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 162 (*cryst struct Cd-form*)

IC-000350

$Al_3F_{14}Na_5$

Pentasodium trialuminium fluoride ($Na_5Al_3F_{14}$)

Tetradecafluorotrialuminate(5−), sodium salt, 8CI

[12068-55-2]

$Na_5Al_3F_{14}$

M 461.8
Tetragonal struct. comprises $Na^{\oplus}$ cations and an $(Al_3F_{14})_n^{5n\ominus}$ layer anion. Synth. by heating a stoichiometric mixture of NaF and AlF_3 (5:3) at 800°. Alternatively produced by reaction of HF with 50% aq. suspension of $Al(OH)_3$ and neutralisation of product with Na_2CO_3. Flux in welding. Colourless tetragonal cryst. ΔH_f° −7581 kJ mol^{-1}; ΔG_f° −7200 kJ mol^{-1}; S° 483.5 J K^{-1} mol^{-1}. Dec. on heating in a peritectic reaction (737°) forming Na_3AlF_6 and liq. of approx. composition 40 mol % AlF_3.

▷ Corrosive; toxic.

Mineral-form [1302-84-7]
Chiolite
Found assoc. with Cryolite in Greenland. Minute cryst.

Brosset, C., *Z. Anorg. Allg. Chem.*, 1938, **238**, 201 (*cryst struct*)
Ginsberg, H. *et al*, *Z. Elektrochem.*, 1957, **61**, 315 (*phase diagram*)
Rolin, M. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 891 (*vp*)
Bondam, J., *Acta Chem. Scand.*, 1971, **25**, 3271 (*ir*)
Cantor, S. *et al*, *Proc. Int. Symp. Molten Salts*, 1976, 417; *CA*, 1978, **89**, 118707 (*synth, thermodynamics*)
Korobitsyn, A.S. *et al*, *Tsvetn. Met.* (*Moscow*), 1984, 51; *CA*, **101**, 173904 (*synth*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 166 (*thermodyn data*)
Kawamoto, Y. *et al*, *J. Non-Cryst. Solids*, 1986, **85**, 335 (*raman*)

IC-000351

$Al_3H_2KO_{12}Si_3$

Muscovite

Common mica. White mica

[1318-94-1]

$K[Al_2(OH)_2Si_3AlO_{10}]$

M 398.3
Mica having double layers with $Al(O,OH)_6$ octahedra between layers of $(Si,Al)O_4$ tetrahedra. $K^{\oplus}$ between double layers. May be made hydrothermally from ammonium aluminosilicate gels. Occurs abundantly as mineral. Colourless plates. Electrical and thermal insulator: used in the manuf. of electrical apparatus. n_D 1.558, 1.594, 1.598.

Radoslovich, E.W., *Acta Crystallogr.*, 1960, **13**, 919 (*cryst struct*)
Barrer, R.M. *et al*, *J. Chem. Soc.*, 1961, 971 (*synth*)
Birke, J.D. *et al*, *Mineral. Mag.*, 1968, **36**, 883 (*cryst struct*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 4889; 1986, **108**, 1730 (*Si-29, Al-27 nmr*)
Sanz, J. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 4790 (*Si-29, Al-27 nmr*)
Mägi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

IC-000352

$Al_3H_3O_{11}P_2$

Aluminium hydroxide phosphate ($Al_3(OH)_3(PO_4)_2$)

[117944-52-2]

$Al_3(OH)_3(PO_4)_2$

M 321.9

Mineral-form [1319-40-0]
Wavellite
Essentially the pentahydrate. Orthorhombic lattice. Alternatively formulated as $Al_3(PO_4)_2(OH,F)_3.5H_2O$. Occurs widely in USA, Brazil, S. Australia; also found in UK, USSR. Easily sol. aq. acids and alkalis. Easily loses H_2O at <200°. Stout, long and brittle. White to greenish-white to green, also yellowish-green to yellow and yellowish-brown, brown to brownish-black prisms.

Mineral-form
Metakingite
Essentially the tetrahydrate.

Mineral-form [12418-34-7]
Kingite
Essentially the nonahydrate. Possibly possesses a kaolinite struct. Alternatively formulated as $Al_3(PO_4)_2(OH,F)_3.9H_2O$. Found at various locations in Australia. White triclinic cryst.

[64535-89-3]

Dana's System of Mineralogy, 7th Ed., Wiley, NY, 1951, 961, 962, 965.
Zamyatin, S.R. *et al*, *Zh. Prikl. Khim.* (*Leningrad*), 1972, **45**, 956; *J. Appl. Chem. USSR* (*Engl. Transl.*), 1972, **45**, 988.
Moreau, J., *Bull. Soc. Fr. Minéral. Cristallogr.*, 1975, **98**, 263.

IC-000353

$Al_3H_4NaO_{12}P_2$

Brazilianite

Aluminium sodium hydroxide phosphate ($Al_3Na(OH)_4(PO_4)_2$)

[12004-65-8]

$NaAl_3(PO_4)_2(OH)_4$

M 361.9
Struct. contains chains of edge-sharing AlO_6 octahedra linked by PO_4 tetrahedra with Na in framework cavities. Mineral. White solid.

Dihydrate: Wardite. Cyrilovite
$Al_3H_8NaO_{14}P_2$ M 397.9
White or coloured cryst. depending on impurities.

Gatehouse, B.M. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 1311 (*cryst struct*)
Hill, F., *Z. Naturforsch., A*, 1978, **33**, 1484 (*esr*)

IC-000354

$Al_2H_6KO_{14}S_2$

Alunite

Potassium hexahydroxybis[sulfato(2−)]trialuminate(1−)

[1302-91-6]

$K[Al_3(OH)_6][SO_4]_2$

M 414.2

Al is coord. by 4OH (at shared corners of AlO_6 octahedra) and $2[SO_4]^{2\ominus}$. Also formulated as $K[Al_3O_3(SO_4)_2].3H_2O$. Obt. from Aluminium sulfate ($Al_2(SO_4)_3$), IC-000328 and aq. KOH. Widely distributed mineral formed by sulfotarız processes on volcanic rocks. Resource for both K and Al. Component of cement. Used in water softening. White cryst. (H_2O). Often discoloured greyish, yellowish, reddish. Na, NH_4, Rb derivs. also descr. Related minerals known with S replaced by P and K by Sr or Ba. Piezoelectric.

[12253-07-5, 12588-67-9]

Bassett, H. *et al, J. Chem. Soc.*, 1949, 2239 (*synth, props*)
Labutin, G.V. *et al, Azerb. Khim. Zh.*, 1962, 95; *CA*, 1963, **59**, 1263a (*synth*)
Wang, R. *et al, Acta Crystallogr.*, 1965, **18**, 249 (*cryst struct*)
Sazhin, V.S. *et al, Zh. Prikl. Khim. (Leningrad)*, 1968, **41**, 1420; *CA*, **69**, 83097 (*synth*)
Wilkins, R.W.T. *et al, Am. Mineral.*, 1974, **59**, 811 (*ir*)
Fedorinenko, I.I. *et al, Khim. Tekhnol. (Kiev)*, 1978, 5; *CA*, 1978, **89**, 95903 (*dta*)
Ripmeester, J.A. *et al, Can. Mineral.*, 1986, **24**, 435 (*pmr*)

IC-000355

$Al_3H_6NaO_{14}S_2$

Aluminium sodium hydroxide sulfate ($Al_3Na(OH)_6(SO_4)_2$)

Hexahydroxybis[sulfato(2−)]trialuminate(1−), sodium salt, 8Cl. Sodium trialuminium hexahydroxide bissulfate

[12377-09-2]

$NaAl_3(OH)_6(SO_4)_2$

M 398.1

Synth. from NaOH + an aq. soln. containing $Al_2(SO_4)_3$ and $MgSO_4$ at 75°. Rhombohedral cryst.

Mineral-form *[12377-08-1]*

Natroalunite

Alternative formulation: $Na[Al_3O_3(SO_4)_2].3H_2O$. Widespread, esp. on volcanic rocks, eg. in Western USA. Rhombohedral colourless to yellowish or reddish cryst.

Moss, A.A. *et al, Mineral. Mag.*, 1958, **31**, 884 (*cryst struct*)
Slansky, E., *Neues Jahrb. Mineral., Monatsh.*, 1973, 124; *CA*, 1974, **80**, 17372 (*dta*)
Danilov, V.P. *et al, Zh. Neorg. Khim.*, 1984, **29**, 1710 (*synth*)
Serna, C.J. *et al, Spectrochim. Acta, Part A*, 1986, **42**, 729 (*ir, raman*)

IC-000356

$Al_3H_{25}O_{27}P_8$

Aluminium hydrogen phosphate ($(H_3O)(Al_3(H_2PO_4)_6(HPO_4)_2).4H_2O$)

$[H_3O][Al_3(H_2PO_4)_6(HPO_4)_2].4H_2O$

M 945.9

AlO_6 octahedra share corners with $O_2P(OH)_2$ and $O_3P(OH)$ tetrahedra to give layers. Synth. from a soln. of $Al^{3\oplus}$ in H_3PO_4 with Al:P 1:4.5 in desiccator over P_2O_5. Colourless cryst. (H_2O).

Erlenmeyer, E., *Justus Liebigs Ann. Chem.*, 1878, **194**, 178 (*synth*)
Brodalla, D. *et al, Z. Naturforsch., B*, 1980, **35**, 403 (*synth, cryst struct*)

IC-000357

$Al_3H_{32}Na_3O_{208}Si_{93}$

Zeolite ZSM-5

$Na_3[Al_3Si_{93}O_{192}].16H_2O$

M 6121.9

Zeolite struct. MFI with 3-D network of two connected sets of channels (530 × 560 and 510 × 550 pm across) with $(Al,Si—O)_{10}$ rings. Member of pentasil group. Synth. from $(Pr_4N)_2O$-$(NH_4)_2O$-Al_2O_3-SiO_2-H_2O mixts. Al-free material (Silicalite) also descr. Catalyst for conversion of MeOH to gasoline, ethylbenzene synth., xylene isomerism and toluene disproportionation. Zeolites ZK1 and ZK2 have similar props.

Flanagan, E.M. *et al, Nature (London)*, 1978, **271**, 512 (*Al-free compd*)
Kokotailo, G.T. *et al, Nature (London)*, 1978, **272**, 437 (*cryst struct*)
Wu, E.L. *et al, J. Phys. Chem.*, 1979, **83**, 2777 (*powder struct*)
Olson, D.H. *et al, J. Phys. Chem.*, 1981, **85**, 2238 (*cryst struct*)
Inorg. Synth., 1983, **22**, 61 (*synth*)
Kentgens, A.P.M. *et al, J. Phys. Chem.*, 1983, **87**, 4357 (*Al-27 nmr*)
Parker, L.M. *et al, Zeolites*, 1983, **3**, 8 (*ZK1 and ZK2*)
Nastro, A. *et al, Zeolites*, 1983, **3**, 57 (*synth*)
Boxhoorn, G. *et al, Zeolites*, 1984, **4**, 15 (*Si-29 nmr*)
Namba, S. *et al, Zeolites*, 1984, **4**, 77 (*absorption props*)
Nagy, J.B. *et al, Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Araya, A. *et al, J. Chem. Res.*, 1985, 192 (*synth*)
Chu, C.T.-W. *et al, J. Phys. Chem.*, 1985, **89**, 1569 (*ir*)
Lerner, H. *et al, Zeolites*, 1985, **5**, 131 (*cryst struct*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 100.
Turro, N.J. *et al, J. Am. Chem. Soc.*, 1987, **109**, 2449 (*use*)
Harrison, I.D. *et al, Zeolites*, 1987, **7**, 21 (*absorption*)
Fyfe, C.A. *et al, J. Am. Chem. Soc.*, 1988, **110**, 3373 (*Si-29 nmr*)
Freude, D. *et al, J. Chem. Soc., Chem. Commun.*, 1988, 1411 (*pmr*)
Ramamurthy, V. *et al, J. Chem. Soc., Chem. Commun.*, 1989, 1213 (*reactions*)
Xu, W. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 755 (*synth*)
Ogawa, H. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 1246 (*use*)
Hutchings, C.J. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 1475 (*use*)
Kim, J.-H. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 1793 (*use*)
Williams, J.H. *et al, J. Chem. Soc., Chem. Commun.*, 1991, 959 (*neutron scattering*)

IC-000358

$Al_3H_{32}Na_3O_{208}Si_{93}$

Zeolite ZSM-11

Pentasil

$Na_3[Al_3Si_{93}O_{192}].16H_2O$

M 6121.9

Zeolite struct. MEL with 3-D network of channels (530 × 540 pm across) with $(Al,Si—O)_{10}$ rings. Member of pentasil group. Made hydrothermally from Na_2O, Al_2O_3, SiO_2, H_2O and a quaternary compd. e.g. Bu_4PCl. Al-free analogue Silicalite 2 also descr.

Kokotailo, G.T. *et al, Nature (London)*, 1978, **275**, 119 (*synth, cryst struct*)
Bibby, D.M. *et al, Nature (London)*, 1979, **280**, 664 (*Al-free compd*)
Nagy, J.B. *et al, Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 94.
Harrison, I.D. *et al, Zeolites*, 1987, **7**, 21 (*absorption*)
Fyfe, C.A. *et al, J. Am. Chem. Soc.*, 1989, **111**, 2470 (*cryst struct*)
Ramamurthy, V. *et al, J. Chem. Soc., Chem. Commun.*, 1989, 1213 (*reactions*)

IC-000359

$Al_3Na_7O_8$

Aluminium sodium oxide ($Al_3Na_7O_8$)

Sodium aluminate ($Na_7(Al_3O_8)$). Heptasodium aluminate ($Al_3O_8^{7\ominus}$)

[79103-36-9]

$Na_7[Al_3O_8]$

M 369.8

Struct. has rings of six AlO_4 tetrahedra linked by two O bridges to form bands. Synth. from Na_2O + Al_2O_3 at 700°. V. hygroscopic white cryst.

Barker, M.G. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 379 (*synth, cryst struct*)

IC-000360

Al_4Ba

Barium aluminium ($BaAl_4$)

Barium aluminium compd. (1:4), 8Cl. Aluminium barium (4:1)

[12253-23-5]

$BaAl_4$

M 245.2

Tetragonal intermetallic compd. Prepd. by fusing together the constituent elements. Used in combination with nickel, as a getter for television tubes. Moisture-sensitive metallic powder. Reacts with H_2O with formn. of H_2 and $Ba(OH)_2$. Dec. on heating to constit. elements. ΔH_f ($BaAl_4$, c, 1215K) −37.1 kJ mol^{-1}; ΔH_f ($BaAl_4$, c, 298K) −123.8 kJ mol^{-1}.

Vigdorovich, V.N. *et al, Zh. Fiz. Khim.*, 1972, **46**, 1426 (*thermal dissoc*)
Bebyakin, M.M. *et al, CA*, 1981, **94**, 143837 (*moisture sensitivity*)
Notin, M. *et al, Thermochim. Acta*, 1982, **57**, 57 (*thermochem data*)
Ger. Pat., 3 523 522, (1986); *CA*, **104**, 160680 (*uses*)
Yarmolyuk, Ya.P., *Kristallografiya*, 1986, **31**, 400 (*cryst struct*)
Zheng, C. *et al, Z. Naturforsch., B*, 1986, **41**, 292 (*electronic struct*)

IC-000361

$Al_4CaH_2O_{12}Si_2$

Margarite

[1318-86-1]

$Ca[Al_2(OH)_2Si_2Al_2O_{10}]$

M 398.1

Brittle mica. Each layer comprises $Al(O,OH)_6$ octahedra between $(Si,Al)O_4$ tetrahedra. $Ca^{2\oplus}$ between layers. Mineral. Platy greyish-pink cryst.

Guggenheim, S. *et al, Am. Mineral.*, 1975, **60**, 1023 (*cryst struct*)
Sanz, J. *et al, J. Am. Chem. Soc.*, 1984, **106**, 4790 (*Al-27, Si-29 nmr*)
Kinsey, R.A. *et al, Am. Mineral.*, 1985, **70**, 537 (*Al-27, Si-29 nmr*)
Lippmaa, E. *et al, J. Am. Chem. Soc.*, 1986, **108**, 1730 (*Al-27 nmr*)

IC-000362

$Al_4CaH_{48}K_2O_{56}Si_{12}$

Erionite

[12510-42-8]

$(Ca,K_2)[Al_2Si_6O_{16}].12H_2O$

M 1507.5

Zeolite struct. ERI with columns of 23 and of 11-hedra, and hexagonal prisms. 3-D channel struct. (360 × 510 pm across) with $(Al,Si—O)_8$ rings. Member of the chabazite group. Also formulated as $(Ca,Mg,Na_2,K_2)_{4.5}[Al_9Si_{27}O_{72}].27H_2O$. Mineral of widespread sedimentary occurrence and in some hydrothermal deposits. Hydrothermal synth. from gels cont. NaOH and $[Me_4N]OH$. Fibrous solid. Void vol. 0.35 cm^3 cm^{-3}.

▷ K.F0115000.

Aiello, R. *et al, J. Chem. Soc. A*, 1970, 1470 (*synth*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, 1974 (*rev*)
Nagy, J.B. *et al, Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Gottardi, G. *et al, Natural Zeolites*, Springer, 1985, 200 (*props*)
Pluth, J.J. *et al, Acta Crystallogr., Sect. C*, 1986, **42**, 283 (*cryst struct*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 58.
Occelli, M.L. *et al, Zeolites*, 1987, **7**, 265 (*synth, catalytic props*)

IC-000363

Al_4CaO_7

Aluminium calcium oxide ($CaAl_4O_7$)

CA_2

[12004-88-5]

$CaAl_4O_7$

M 260.0

Struct. comprises linked AlO_4 distorted tetrahedra with 7-coord. Ca. Synth. from $CaCO_3$ + Al_2O_3 at 1800°. Host for $Nd^{3\oplus}$ as laser material. Colourless needles (from melt). Mp 1745°. ΔH_f° −3977.7 kJ mol^{-1}; S° 188.7 J K^{-1} mol^{-1}. Sr analogue also descr.

Boyko, E.R. *et al, Acta Crystallogr.*, 1958, **11**, 444 (*synth, cryst struct*)
Nurse, R.W. *et al, Trans. Brit. Ceram. Soc.*, 1965, **64**, 409 (*phase diagram*)
Cockayne, B., *J. Am. Ceram. Soc.*, 1966, **49**, 204 (*synth*)
Rao, M.R. *et al, J. Am. Ceram. Soc.*, 1968, **51**, 50 (*phase diagram*)
Oudalov, Y.P. *et al, Mater. Res. Bull.*, 1969, **4**, 887 (*synth*)
Goodwin, D.W. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 1230 (*synth, cryst struct*)
Ponomarev, V.I., *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1970, **15**, 995 (*cryst struct*)
Allibert, M. *et al, J. Am. Ceram. Soc.*, 1981, **64**, 307 (*thermodyn data*)
Eliezer, I. *et al, J. Phys. Chem.*, 1981, **85**, 2835 (*thermodyn data*)
Müller, D. *et al, Polyhedron*, 1986, **5**, 779 (*Al-27 nmr*)

IC-000364

$Al_4Ca_2H_{24}O_{48}Si_{14}$

Heulandite

[1318-63-4]

$Ca_2[Al_4Si_{14}O_{36}].12H_2O$

M 1373.4

Zeolite struct. HEU with Si:Al < 4 comprises system with 1D channels 330 × 460 and 260 × 470 pm across of $(Al,Si—O)_8$ rings and channels (300 × 760 pm across) of $(Al,Si-O)_{10}$ rings. Sedimentary mineral. Occurs chiefly in basalts and andesites in Iceland, Nova Scotia, New Zealand and elsewhere. Hydrothermal synth. from gels at 250-450°. Tabular pearly white cryst.

Merkle, A.B. *et al, Am. Mineral.*, 1967, **52**, 273; 1968, **53**, 1120 (*cryst struct*)
Lippmaa, E. *et al, J. Am. Chem. Soc.*, 1981, **103**, 4992 (*Si-29 nmr*)
Barrer, R.M., *Hydrothermal Chemistry of Zeolites*, Academic Press, London, 1982.
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 72.

IC-000365

$Al_4Ca_4H_8O_{30}Si_8$

Roggianite, 9Cl

[12511-82-9]

$Ca_4H_8[(Al_4Si_8)O_{36}](OH)_4 \sim 6.5H_2O$

$Al_6Ca_{16}FeH_4MgO_{88}Si_9$

Vesuvianite, 9CI IC-000366

Idocrase

[1319-37-5]

$Ca_{10}(Mg,Fe)_2Al_4[SiO_4]_5[Si_2O_7]_2(OH)_4$

M 1453.6

Mineral. Complex orthosilicate with both SiO_4 and Si_2O_7 groups. Ca 8-coord. Al, Mg, Fe 5- or 6-coord. Commonly occurs in metamorphosed limestones in widespread locations. A minor gem stone. Cryst. of various colours including green, brown, white, yellow, red, purple.

Rucklidge, J.C. *et al, Can. Mineral.*, 1975, **13**, 110 (*cryst struct*)
Manning, P.G. *et al, Can. Mineral.*, 1975, **13**, 259.
Manning, P.G. *et al, J. Inorg. Nucl. Chem.*, 1981, **43**, 1169 (*Mössbauer*)
Deer, W.A. *et al, Rock Forming Minerals*, 2nd Ed., Longman, London, 1982, **1A**, 699.

$Al_4H_8O_{18}Si_4$

Halloysite IC-000367

[12068-50-7]

$Al_2Si_2O_5(OH)_4$

M 516.3

Struct. has irregular sequence of kaolin layers each with net of SiO_4 tetrahedra and $Al(O,OH)_6$ octahedra. Common clay mineral; various hydrated forms known. Natural hydrated form, but not dehydrated form Metahalloysite, adsorbs variety of org. alcohols, ethers, nitriles. Catalyst for hydrorefining and hydrogenation. White to grey or brown solid. Ion exchange capacity 0.05 to 0.5 eq kg^{-1}.

MacEwan, D.M.C., *Trans. Faraday Soc.*, 1948, **44**, 349 (*cryst struct, props*)
Van Olpen, H., *Clay Colloid Chemistry*, Wiley, 2nd Ed., 1977 (*rev, props*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **6**, 190 (*rev*)
Borovec, Z., *CA*, 1981, **94**, 181286 (*ion exchange*)

Al_4Li_9

Aluminium compd. with lithium (4:9) IC-000368

Aluminium lithium (Al_4Li_9). Lithium aluminium (Li_9Al_4). Alumtnium compd. with lithium (1:2) (incorr.)

[12253-44-0]

Al_4Li_9

M 170.3

Formerly descr. as Li_2Al. Struct. has zig-zag Al_n chains with Li's between. Each atom has coord. no. 14. Synth. from the elements at 500°. Moisture sensitive cryst. (melt).

Hansen, D.A. *et al, Acta Crystallogr., Sect. B*, 1968, **24**, 913 (*cryst struct*)

$Al_4Na_4O_{18}Si_5$

Zeolite X IC-000369

$Na_4[Al_4Si_5O_{18}]$

M 628.3

Zeolite struct. FAU with Si:Al 1-1.5. Important synthetic zeolite, aluminous form of Faujasite, IC-000257. Many ion exchanged forms known (Ag, Ba, Ca, Ce, Cu, Hg, Na, Pb, Tl etc.). Synth. from aq. $NaAlO_2$, sodium silicate, SiO_2 and NaOH at 20-120°. Ion exchanger; shape-selective catalyst; drying agent. Host for alkali metal clusters. Stable white solid; reversibly dehydrates. Void volume 0.5 cm^3cm^{-3}.

Broussard, L. *et al, J. Am. Chem. Soc.*, 1960, **82**, 1041 (*cryst struct*)
Olsen, D.H., *J. Phys. Chem.*, 1970, **74**, 2758 (*cryst struct*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, N.Y., 1974 (*props, synth, use*)
Lippmaa, E. *et al, J. Am. Chem. Soc.*, 1986, **108**, 1730 (*Al-27 nmr*)
Engelhardt, G. *et al, High Resolution Solid State NMR of Silicates and Zeolites*, Wiley, 1987 (*Si-29 nmr*)
Anderson, P.A. *et al, J. Chem. Soc., Chem. Commun.*, 1991, 914, 915 (*use*)

$Al_4O_{32}Si_{12}Sr_2$

Brewsterite IC-000370

[12197-41-0]

$Sr_2[Al_2Si_{12}O_{32}].10H_2O$

M 1132.1

Zeolite struct. BRE; a member of Heulandite group Sr 9-coord. Layer struct. with two interconnected 1D channels (230 × 500 and 280 × 410 pm) between layers. Rare zeolite from cavities of basaltic rocks. Extensive replacement Sr by Ca and Ba. Layer struct. with two interconnected 1D channels (230 × 500 and 280 × 410 pm) between layers. Colourless platy cryst. Adsorbs water but not other small molecules. Void vol. 0.26 cm^3 cm^{-3}.

Perrotta, A.J. *et al, Acta Crystallogr.*, 1964, **17**, 857 (*cryst struct*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, N.Y, 1974, 130, 137, 211.
Schlenker, J.L. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2907 (*cryst struct*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 38.
Dyer, A., *Introduction to Zeolite Molecular Sieves*, Wiley, N.Y, 1988, 42 (*nd*)

$Al_5H_6MgNaO_{36}Si_{12}$

Montmorillonite IC-000371

[1318-93-0]

$Na[Al_5MgSi_{12}O_{30}(OH)_6]$

M 1101.2

Struct. has Pyrophyllite, IC-000289 double layers with replacement of some octahedral $Al^{3\oplus}$ by $Mg^{2\oplus}$ and interlayer $Na^{\oplus}$ and H_2O. Widely distributed clay mineral. Adsorbs range of org. compds. esp. alcohols, glycols, ketones, nitriles. Modified pillared forms used as shape-selective catalysts. Dull white, grey, yellowish, greenish or pink solid. Vol. increased several fold by adsorption of H_2O. Cation exchange capacity 0.6-1.5 eq kg^{-1}.

MacEwan, D.M.C., *Trans. Faraday Soc.*, 1948, **44**, 349 (*cryst struct, complexes*)
MacKenzie, R.C., *Trans. Faraday Soc.*, 1948, **44**, 368 (*complexes*)
Barrer, R.M. *et al, J. Chem. Soc.*, 1961, 971 (*synth*)

Van Olpen, H., *Introduction to Clay Colloid Chemistry*, 2nd Ed., Wiley, N.Y., 1977 (*rev, props*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 23; **6**, 197 (*rev, uses*)
Smith, K.A. *et al, Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)
Kinsey, R.A. *et al, Am. Mineral.*, 1985, **70**, 537 (*Al-27, Si-29 nmr*)
Tennakoon, D.T.B. *et al, J. Chem. Soc., Faraday Trans. 1*, 1986, **82**, 545 (*Al-27, Si-29 nmr*)
Tichit, D. *et al, Clays Clay Miner.*, 1988, **36**, 369 (*pillared form*)
González, F. *et al, J. Chem. Soc., Chem. Commun.*, 1991, 587 (*pillared form*)

$Al_5KMg_2O_{30}Si_{10}$

Osumilite IC-000372

[12420-38-1]

$KMg_2Al_3[(Al_2Si_{10})O_{30}]$

M 983.4

Unbranched, dicyclosilicate. Also formulated as $(K,Na)(Mg,Fe)_2(Al,Fe)_3(Si,Al)_{12}O_{30}.1H_2O$. Mineral. Blue to black cryst.

Schreyer, W. *et al, Contrib. Mineral. Petrol.*, 1967, **14**, 343 (*synth*)
Brown, G.E., *Am. Mineral.*, 1969, **54**, 101 (*cryst struct*)
Sandanirskii, P.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1978, **238**, 851 (*cryst struct*)
Povarennykh, A.S., *Mineral. Zh.*, 1979, **1**, 3 (*ir*)
Hesse, K.-F. *et al, Z. Kristallogr.*, 1982, **160**, 179 (*cryst struct*)
Hemingway, B.S. *et al, Am. Mineral.*, 1984, **69**, 701.

Al_5NaO_8

Aluminium sodium oxide (Al_5NaO_8) IC-000373

β″-Alumina

[12005-16-2]

$Na[Al_5O_8]$

M 285.8

Composition variable. Also designated $NaAl_6O_8$. Spinel-like layers 1120 pm thick with Na between (see also Aluminium sodium oxide ($Al_{11}NaO_{17}$), IC-000395). Synth. from solid state reaction between Al_2O_3 + Na_2CO_3 at 1050°. White solid.

Thery, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1962, **254**, 2782 (*synth*)
Scholder, R. *et al, Z. Anorg. Allg. Chem.*, 1963, **321**, 246 (*synth*)
Yamaguchi, G. *et al, Bull. Chem. Soc. Jpn.*, 1968, **41**, 93 (*synth, cryst struct*)
de Vries, R.C. *et al, J. Am. Ceram. Soc.*, 1969, **52**, 364 (*rev*)
Bettman, M. *et al, J. Phys. Chem.*, 1969, **73**, 1774 (*synth, cryst struct*)

$Al_5Na_{17}O_{16}$

Aluminium sodium oxide ($Al_5Na_{17}O_{16}$) IC-000374

Heptadecasodium aluminate ($Al_5O_{16}^{17\ominus}$), 11Cl. Sodium aluminate ($Na_{17}(Al_5O_{16})$)

[83118-07-4]

$Na_{17}[Al_5O_{16}]$

M 781.7

AlO_4 tetrahedra share corners to give Al_5O_{16} chains. Synth. from solid state reaction between Na_2O and α-Al_2O_3 at 700°. V. hygroscopic white solid.

Barker, M.G. *et al, J. Chem. Soc., Chem. Commun.*, 1982, 516 (*cryst struct*)

$Al_5O_{12}Y_3$

Aluminium yttrium oxide ($Al_5Y_3O_{12}$) IC-000375

Yttrium aluminium garnet. YAG. Pentaaluminium triyttrium dodeca oxide

[12005-21-9]

$Y_3Al_2(AlO_4)_3$

M 593.6

Cubic garnet struct. Obt. from the melted oxide or hydrothermal synth. from Y_2O_3, Al_2O_3, in 6*M* aq. K_2CO_3. Laser host material. When $Ce^{3\oplus}$-activated, used in flying-spot scanner for colour TV signals. $Nd^{3\oplus}$ doped for laser applications. Used to make artificial diamonds. Colourless cryst. (melt). Mp 1980° (1970°). Several related phases descr. n_D 1.835. Gd analogue also descr. $Y_4Al_2O_9$, $YAlO_3$ also descr.

[88506-07-4]

Bertaut, M. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1956, **243**, 1219.
Van Hook, H.J., *J. Am. Ceram. Soc.*, 1963, **46**, 121 (*synth*)
Gensic, I.E., *Appl. Phys. Lett.*, 1964, **4**, 182 (*use*)
Cockayne, B., *J. Am. Ceram. Soc.*, 1966, **49**, 204 (*synth*)
Tarte, P., *Spectrochim. Acta, Part A*, 1967, **23**, 2127 (*ir*)
Bril, A. *et al, Phillips Tech. Rev.*, 1971, **32**, 125 (*use*)
Messier, D.R. *et al, Am. Ceram. Soc. Bull.*, 1972, **51**, 692 (*synth*)
Liebetz, J., *Angew. Chem., Int. Ed. Engl.*, 1973, **12**, 291 (*rev*)
Nekvasil, V. *et al, Czech. J. Phys.*, 1974, **24**, 810 (*Nd, magnetism*)
Abell, J.S. *et al, J. Mater. Sci.*, 1974, **9**, 527 (*phase diagram*)
Kolb, E.D. *et al, J. Crystal Growth*, 1975, **29**, 29 (*synth*)
Emraliev, A. *et al, Kristallografiya*, 1976, **21**, 211 (*cryst struct*)
Danielmeyer, H.G., *Lasers*, (Lavine A.K. *et al*, Ed.) Marcel Dekker, 1976, **4**, 1 (*rev, uses*)
Akhmetov, S.F. *et al, Zh. Neorg. Khim.*, 1977, **26**, 2966; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1977, **22**, 1613 (*synth, props, tga*)
Shishido, T. *et al, J. Am. Ceram. Soc.*, 1978, **61**, 373 (*Gd analogue*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **11**, 721; **19**, 852 (*use*)
Valentich, J., *J. Mater. Sci.*, 1979, **14**, 371 (*thermal props*)
Bates, J.L. *et al, J. Am. Ceram. Soc.*, 1981, **64**, C138 (*elec cond*)

$Al_{5.2}Ca_{1.1}H_{30.4}K_{1.1}Mg_{0.7}O_{51.2}Si_{12.8}$

Offretite IC-000376

[12417-81-1]

$(Ca,Mg)_{1.5}K[Al_4Si_{14}O_{36}].14H_2O$ or
$(K_2,Ca,Mg)_{2.5}[(AlO_2)_5(SiO_2)_{13}].15H_2O$

M 1453.7

Zeolite struct. OFF. Member of chabazite group. Struct. composed of 2 types of 14-hedra and alternating 11-hedra and hexagonal prisms, with three of each round each wide channel. Struct. contains 1D circular channels (670 pm across) perpendicular and interconnected to 2D channnels (360 × 490 pm across). Mineral found in cavities of basaltic rocks in France, USA, Germany and Australia. Synth. from Al_2O_3—SiO_2—H_2O mixt. + $(Me_4N)_2O$, $H_2N(CH_2)_2NH_2$ or $H_2N(CH_2)_2OH$. Colourless hexagonal prisms.

Me_4N form: White solid (H_2O).

Aiello, R. *et al, J. Chem. Soc. A*, 1970, 1470 (*synth*)
Gard, J.A. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 825 (*cryst struct*)
Inorg. Synth., 1983, **22**, 61 (*synth*)
Nagy, J.B. *et al, Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Fyfe, C.A. *et al, Zeolites*, 1985, **5**, 179 (*Al-27, Si-29 nmr*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 114.
Howden, M.G., *Zeolites*, 1987, **7**, 255, 260.
Moudafi, L. *et al, Zeolites*, 1987, **7**, 63 (*synth*)
Occelli, M.L. *et al, Zeolites*, 1987, **7**, 265 (*synth, catalytic props*)

$Al_6AsH_6Mn_4O_{28}Si_5$ IC-000377

Ardennite, 9Cl

[12211-29-9]

$$Mn_4Al_6[(As,V)O_3][SiO_4]_2[Si_3O_{10}](OH)_6$$

M 1051.0

Rare mineral. Also formulated as $Mn_4(Al,Mg)_6(SiO_4)_2(Si_3O_{10})[(As,V)O_4](OH)_6$. Found in veins and pegmatites, in the Ardennes, Belgium and in the Piedmont, USA. Yellow to brown orthorhombic prisms.

Winchell, A.N. *et al, Elements of Optical Mineralogy, Part II*, 4th Ed., Wiley, N.Y., 1951, 529.
Senet, J. *et al, Ann. Soc. Geol. Belg.*, 1965, **88**, 545 (*mineral*)
Donnay, G. *et al, Acta Crystallogr., Sect. B*, 1968, **24**, 845 (*cryst struct*)
Reinecke, T. *et al, Neues Jahrb. Mineral., Abh.*, 1987, **158**, 89 (*occur*)

$Al_6B_3FFe_2NaO_{30}Si_6$ IC-000378

Buergerite

[12043-63-9]

$$NaFe_3Al_6B_3Si_6O_{30}F$$

M 1052.3

An example of the Tourmaline group of trigonal borosilicate minerals of general formula $WX_3Y_6(BO_3)_3Si_6O_{18}(O,OH,F)_4$, where W = Ca, K, Na; X = Al, Fe^{II}, Fe^{III}, Li, Mg, Mn^{II} and Y = Al, Cr^{III}, Fe^{III}, V^{III}. Struct. has BO_3 triangles and rings of 6 SiO_4 tetrahedra joined by corners. Short prisms. Colour ranges from black for high Fe specimens to colourless for high Mg. Other minerals in the group include Dravite, Schorl, Elbaite and Uvite.

[1317-93-7]

Donnay, G. *et al, Acta Crystallogr.*, 1950, **3**, 379 (*cryst struct*)
Buerger, M.J. *et al, Acta Crystallogr.*, 1962, **15**, 583 (*cryst struct*)
Mason, B. *et al, Science (Washington, D.C.)*, 1964, **144**, 71 (*rev, props*)
Barton, R., *Acta Crystallogr., Sect. B*, 1969, **25**, 1524 (*cryst struct*)
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)
Encyclopedia of Minerals, Roberts, W.L., *et al*, Eds., 2nd Ed., Van Nostrand Reinhold, 1990, 879.

$Al_6BaCa_2H_4O_{31}Si_9$ IC-000379

Armenite, 9Cl

[12418-15-4]

$$BaCa_2Al_6[Al_2Si_9O_{30}].2H_2O$$

M 1132.1

Mineral. A rare double-ring silicate of the milarite group. Occurs near Kongsberg, Norway and at Remigny, Quebec. Greyish green, translucent trigonal prisms.

Tennyson, C., *Neues Jahrb. Mineral., Abh.*, 1960, **94**, 1253 (*occur, struct*)
Balakin, V.V. *et al, Kristallografiya*, 1974, **19**, 741; *CA*, **81**, 142495m (*cryst struct*)
Pouliot, G. *et al, Can. Mineral.*, 1984, **22**, 453 (*occur, mineral*)

$Al_6Ca_2H_{24}K_2Na_4O_{44}Si_{10}$ IC-000380

Phillipsite

[12174-18-4]

$$K_2(Ca_2Na_4)[Al_6Si_{10}O_{32}].12H_2O$$

M 1421.2

Zeolite struct. PHI of cross linked chains with three sets of interconnected channels (360, 300 × 430 and 320 × 330 pm across) all with $(Si,Al—O)_8$ rings. Synth. from aluminosilicate glass with Na,K,Ca at 250°, or (with phosphate) at 100°. Mineral occurs widely esp. under oceans. Short prismatic white cryst. Related to harmotone. Barian variety known as Wellsite.

Steinfink, H., *Acta Crystallogr.*, 1962, **15**, 644 (*cryst struct*)
Kuhl, G.H., *Am. Mineral.*, 1969, **54**, 1607 (*synth*)
Rinaldi, R. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 2426 (*cryst struct*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, 1974.
Wirsching, U., *Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Gottardi, G. *et al, Natural Zeolites*, Springer, Berlin, 1985, 134.
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 120.

$Al_6Ca_4O_{13}$ IC-000381

Aluminium calcium oxide ($Al_6Ca_4O_{13}$)

C_4A_3

[12421-41-9]

$$Ca_4O[Al_6O_{12}]$$

M 530.1

Cubic structure related to Sodalite, IC-000344 with identical AlO_4 tetrahedra linked to give cubooctahedra joined in infinite framework with $(AlO)_6$ rings and OCa_4 tetrahedra in cavities. Synth. from oxide melt. White cryst. Compds. with other anions in place of $O^{2\ominus}$ descr.

Ponomarev, V.I. *et al, Sov. Phys. Crystallogr. (Engl. Transl.)*, 1970, **15**, 799 (*cryst struct*)
Imlach, J.A. *et al, Trans. Brit. Ceram. Soc.*, 1973, **72**, 221 (*syst with FeO*)
Depmeir, W., *J. Appl. Crystallogr.*, 1979, **12**, 623 (*cryst struct, analogue*)
Depmeir, W., *Acta Crystallogr., Sect. C*, 1984, **40**, 226 (*cryst struct*)
Müller, D. *et al, Polyhedron*, 1986, **5**, 779 (*Al-27 nmr*)

$Al_6Ca_5O_{14}$ IC-000382

Aluminium calcium oxide ($Al_6Ca_5O_{14}$)

C_5A_3

[12005-26-4]

$$Ca_5[Al_6O_{14}]$$

M 586.2

Structure has twisted sheets of distorted AlO_4 tetrahedra linked by corners, with 6-coord. Ca in between. Synth. from oxide melt. White cryst. (melt). Ternary systems with CaO, MgO also descr.

Nurse, R.W. *et al, Trans. Brit. Ceram. Soc.*, 1965, **64**, 409 (*phase diagram*)
Eremin, N.I., *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1973, **9**, 1241; **10**, 96 (*phase diagram*)
Chemekova, T.Yu. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, **10**, 2191 (*synth*)
Vincent, M.G. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 1422 (*cryst struct*)
Müller, D. *et al, Polyhedron*, 1986, **5**, 779 (*Al-27 nmr*)

$Al_6H_{36}Mg_2Na_2O_{90}Si_{30}$ IC-000383

Ferrierite

Zeolite ZSM-35

[12173-30-7]

$$Na_2Mg_2[Al_6Si_{30}O_{72}].18H_2O \text{ or } (Na,K)_2MgAl_3Si_{15}O_{36}(OH).9H_2O$$

M 2575.2

Member of mordenite group. Zeolite struct. FER comprises sheets of $(Al,Si)O_4$ tetrahedra linked by $(Al,Si-O)_6$ rings giving 1D channels of $(Al,Si-O)_{10}$ rings (420 × 540 pm across) and $(Al,Si-O)_8$ rings (350 × 480 pm across). Na, Mg variable. Hydrothermal synth. in presence of en or CO_2 at 390°. Mineral from USA, Canada, Italy, Germany, USSR and Australia. Used as catalyst for hydrocarbon cracking and desulfurisation. White needles. Void vol. 0.28 cm^3 cm^{-3}. ZSM-48 has related struct.

Barrer, R.M. *et al, J. Chem. Soc.*, 1964, 485 (*synth*)
Barrer, R.M. *et al, Am. Mineral.*, 1965, **50**, 484 (*synth*)
Vaughan, P.A., *Acta Crystallogr.*, 1966, **21**, 983 (*cryst struct*)
Hawkins, D.M., *Mater. Res. Bull.*, 1967, **2**, 951 (*synth*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, London, 1973 (*props*)
Cormier, W.E. *et al, Am. Mineral.*, 1976, **61**, 1259 (*synth*)
U.S. Pat., 4 016 245, (1977); *CA*, **86**, 178180 (*synth, use*)
Fyfe, C.A. *et al, J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Townsend, P.R. *et al, Zeolites*, 1984, **4**, 191 (*ion exch props*)
Gramlich-Meir, R. *et al, Am. Mineral.*, 1985, 70, 619 (*cryst struct*)
Araya, A. *et al, J. Chem. Res.*, 1985, 192 (*synth*)
Gottardi, G. *et al, Natural Zeolites*, Springer, 1985, 244.
Schlenker, J.L. *et al, Zeolites*, 1985, **5**, 355 (*ZSM-48*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 64.
Harrison, I.D. *et al, Zeolites*, 1987, **7**, 21 (*adsorption*)
Loizidou, M. *et al, Zeolites*, 1987, **7**, 153 (*ion exch props*)

$Al_6H_{48}Na_6O_{96}Si_{30}$ IC-000384

Clinoptilolite

[12173-10-3]

$$Na_6[Al_6Si_{30}O_{72}].24H_2O \text{ or } (Na,K,Ca)_6(Si,Al)_{36}O_{72}.20H_2O$$

M 2726.7

Probably alkali rich Zeolite struct. HEU with Si : Al >4. Comprises two interconnected 1D channels (260 × 470 and 300 × 760 pm) and further 1D channel 330 × 460 pm. Zeolite struct. CLI. Member of heulandite group. Mineral of extensive sedimentary occurrence in USA, Australia and New Zealand. Synth. from $Al_2O_3—SiO_2—Na_2O—H_2O$ gel at 200-250°. Important ion exchanger in water purification, nuclear waste processing and an industrial catalyst. Platy white solid. Void fract. 0.34.

Mumpton, F.A., *Am. Mineral.*, 1960, **45**, 351 (*powder struct, props*)
Hawkins, D.B., *Mater. Res. Bull.*, 1967, **2**, 951 (*synth*)
Wise, W.S. *et al, Am. Mineral.*, 1969, **54**, 887 (*props*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, N.Y., 1973, 139.
Koyama, K. *et al, Z. Kristallogr.*, 1977, **145**, 216 (*props*)
Nagy, J.B. *et al, Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Townsend, R.P. *et al, Zeolites*, 1984, **4**, 191 (*ion exch props*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 72.
Loizidou, M. *et al, Zeolites*, 1987, **7**, 153 (*ion exch*)

$Al_6O_{13}Si_2$ IC-000385

Mullite

[1302-93-8]

$$Al_6Si_2O_{13}$$

M 426.0

Struct. contains disordered $(Si,Al)O_4$ tetrahedra and AlO_6 octahedra. Widely distributed mineral. Synthetic samples form from oxide melts or from monophasic or diphasic gels. Important refractory. Colourless to pale pink.

Agrell, S.O. *et al, J. Am. Ceram. Soc.*, 1960, **43**, 69 (*cryst struct, optical data*)
Holm, J.L. *et al, Am. Mineral.*, 1966, **51**, 1608 (*thermodyn*)
Askay, I.A., *J. Am. Ceram. Soc.*, 1975, **58**, 507 (*phase diagram*)
Bullens, M. *et al, J. Am. Ceram. Soc.*, 1978, **61**, 81 (*esca, fluorescence*)
Howald, R.A. *et al, J. Phys. Chem.*, 1978, **82**, 2199 (*thermodyn*)
Thomas, J.M. *et al, Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 614 (*Al-27, Si-29 nmr*)
Hoffman, D.W. *et al, J. Am. Ceram. Soc.*, 1984, **67**, 468 (*synth*)
Komarneni, S. *et al, J. Am. Ceram. Soc.*, 1985, **68**, C243 (*Al-27 nmr*)

$Al_8Ba_4Ca_2H_4Na_2O_{54}S_3Si_{12}$ IC-000386

Wenkite

[12178-61-9]

$$Ba_4Ca_2Na_2[Al_8Si_{12}O_{39}(OH)_2](SO_4)_3.H_2O$$

M 2192.5

Zeolite struct. WEN with 2D channel (260 × 490 pm across) having $(Al,Si—O)_{10}$ rings connected to 1D channel (220 × 270 pm across) having $(Al,Si—O)_8$ rings. Mineral found in Italian marbles. Light grey prisms.

Wenk, H.-R., *Z. Kristallogr.*, 1973, **137**, 113.
Merlino, S., *Acta Crystallogr., Sect. B*, 1974, **30**, 1262 (*cryst struct*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 136.

$Al_8H_{48}Na_8O_{60}Si_{16}$ IC-000387

Gmelinite

Groddeckite

[12251-35-3]

$$Na_8[Al_8Si_{16}O_{48}].24H_2O$$

M 1857.4

Zeolite struct. GME with 3D channel system with stacking faults partly blocking channels parallel to *c* axis (700 pm diameter with $(Al,Si—O)_{12}$ and 360 × 390 pm diameter with $(Al,Si—O)_8$ rings). From silica sol + aminepolymer + $NaAlO_2$ at 90°. Mineral found in basaltic lavas and related igneous rocks in USA, Canada, Ireland, Australia and elsewhere. Tabular white cryst.

Aiello, R. *et al, J. Chem. Soc. A*, 1970, 1470 (*synth*)
U.S. Pat., 4 061 717, (1977); *CA*, **88**, 111076.
Daniels, R.H. *et al, J. Am. Chem. Soc.*, 1978, **100**, 3097 (*synth*)
Lippmaa, E. *et al, J. Am. Chem. Soc.*, 1981, **103**, 4992; 1986, **108**, 1730 (*Si-29 nmr, Al-27 nmr*)
Fyfe, C.A. *et al, J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 68.
Davis, M.E. *et al, J. Chem. Soc., Chem. Commun.*, 1988, 920 (*synth*)

$Al_8Na_8O_{96}Si_{40}$ IC-000388

Mordenite

Ptilolite

[12173-98-7]

$$Na_8(Al_8Si_{40}O_{96}).24H_2O$$

M 3059.1

Zeolite struct. MOR comprises puckered hexagonal sheets of $(Al,Si)O_4$ tetrahedra connected through $(Si,Al-O)_4$ rings to give two inter-connected sets of 1D channels, one 650 × 700 pm with $(Si,Al-O)_{12}$ rings and the other 260 × 570 pm with $(Si,Al-O)_8$ rings. Mineral occurs in veins and cavities in igneous rocks as a hydration product of glasses and as an authigenic deposit in sediments. Found in USA, Canada, Italy, Iceland,

Scotland, USSR, Japan and elsewhere. Hydrothermal synth. from gels at 300-415° and 1-3 × 10^3 atm. White cryst. (aq. melt). Many ion exchanged forms known: Ag, Ba, Ca, Cr, K, Li, NH_4 etc.

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1948, 2158; 1952, 1561; 1959, 195 (*synth, ion exch, powder struct*)
Meier, W.M., *Z. Kristallogr.*, 1961, **115**, 439 (*cryst struct*)
Hawkins, D.B., *Mater. Res. Bull.*, 1967, **2**, 951 (*synth*)
Daniels, R.H. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3097 (*synth*)
Fyfe, C.A. *et al*, *J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Klinowski, J. *et al*, *Zeolites*, 1983, **3**, 5 (*Si-29, Al-27 nmr*)
Pechar, F. *et al*, *Zeolites*, 1983, **3**, 329 (*ir*)
Nambar, S. *et al*, *Zeolites*, 1984, **4**, 77 (*absorption*)
Nagy, J.B. *et al*, *Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Townsend, P.R. *et al*, *Zeolites*, 1984, **4**, 191 (*ion exch props*)
Hays, G.R. *et al*, *Zeolites*, 1984, **4**, 377 (*Si-29 nmr*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 1730 (*Al-27 nmr*)
Bajpai, P.K., *Zeolites*, 1986, **6**, 2 (*synth, rev*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 102.
Loizidou, M. *et al*, *Zeolites*, 1987, **7**, 153 (*ion exch props*)
Davis, M.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 920 (*synth*)
Enzel, P. *et al*, *J. Phys. Chem.*, 1989, **93**, 6270 (*use*)

$Al_9Fe_2HO_{24}Si_4$ IC-000389

Staurolite

[12182-56-8]

$HFe_2AlO_4[Al_2SiO_5]_4$

M 851.8

Orthosilicate in which SiO_4 tetrahedra share edges. H, Al, octahedrally and Al, Fe tetrahedrally coord. Blocks in struct. similar to Kyanite, IC-000326. Mineral, assoc. with Kyanite, IC-000326 in schists. Used to make ornaments. Short prismatic dark brown or reddish brown cryst. with uncoloured to greyish streak.

[63043-12-9]

Náray-Szabó, I. *et al*, *Acta Crystallogr.*, 1958, **11**, 862 (*cryst struct*)
Regnard, J.R., *J. Phys. Colloq.*, 1976, 797 (*mössbauer*)
Scorzelli, R.B. *et al*, *J. Phys. Colloq.*, 1976, 801 (*mössbauer*)
Hunt, G.R., *Geophysics*, 1977, **42**, 501 (*ir*)
Gibbons, K. *et al*, *Mineral. Mag.*, 1981, **44**, 69 (*powder struct*)
Lefebvre, A., *Phys. Chem. Miner.*, 1982, **8**, 251 (*lattice defects*)
Tagai, T. *et al*, *Neues Jahrb. Mineral., Monatsh.*, 1985, 97 (*nd*)
Varma, H.V. *et al*, *Phys. Status Solidi A*, 1986, **97**, 275 (*mössbauer*)

$Al_9Mn_3Si_5$ IC-000390

Aluminium manganese silicide ($Al_9Mn_3Si_5$)

Manganese aluminium silicide

$Al_9Mn_3Si_5$

M 548.0

Hexagonal struct. related to Co_2Al_5. Mn-Al distance of 242 pm suggests electron transfer from Al to Mn. Prepd. from melt. Effective deoxidising agent for steel. Useful in studying creep behaviour of Al alloys. Bluish-grey tinted cryst. Cryst. irregularly attacked by acids and alkalies. The phases $Al_{12}Mn_3Si$, $MnAl_{0.75}Si_{1.25}$ and Mn_3AlSi_5 also exist.

Phillips, H.W.L., *J. Inst. Met.*, 1945, **69**, 275 (*synth*)
Robinson, K., *Acta Crystallogr.*, 1952, **5**, 397 (*synth, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **C8**, 107 (*rev, bibl*)

$Al_9Na_9O_{48}Si_{15}$ IC-000391

Zeolite ZK-4

$Na_9[Al_9Si_{15}O_{48}]$

M 1638.9

Zeolite struct. LTA. Structural isotype of Zeolite A, IC-000398 but with higher Si:Al ratio. Member of faujasite group. Synth. from sodium aluminate, SiO_2, Me_4NOH and H_2O at 100°. Adsorbs straight chain hydrocarbons. White cryst. (aq. melt).

Kerr, G.T. *et al*, *Inorg. Chem.*, 1966, **5**, 1537 (*synth*)
Thomas, J.M. *et al*, *J. Phys. Chem.*, 1982, **86**, 3061 (*Si-29 nmr*)
Eddy, M.M. *et al*, *Zeolites*, 1986, **6**, 449 (*nd*)
Thangaraj, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1991, 493 (*N-14 nmr*)

$Al_{10}Ca_4Na_2O_{72}Si_{27}$ IC-000392

Stilbite

[12174-59-3]

$Na_2Ca_4[Al_{10}Si_{27}O_{72}].28H_2O$

M 2386.3

Member of heulandite group, Zeolite struct. STI. Layer struct. with channels 490 × 610 pm with $(Al,Si—O)_{10}$ rings connected to 1D channels (270 × 560 pm) with $(Al,Si—O)_8$ rings. Mineral: natural zeolite occuring in basalts. Found in USA, Brazil, Poland, New Zealand and elsewhere. Twinned lamellar colourless cryst. Wide variations in stoichiometry. Related Stellerite and Barrerite also descr.

Galli, E., *Acta Crystallogr., Sect. B*, 1971, **27**, 833 (*cryst struct*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4992 (*Si-29 nmr*)
Nagy, J.B. *et al*, *Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Gottardi, G. *et al*, *Natural Zeolites*, Springer, Berlin, 1985, 284.
Miller, S.A. *et al*, *Zeolites*, 1985, **5**, 7 (*nd*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 130.
Quartieri, S. *et al*, *Zeolites*, 1987, **7**, 163 (*cryst struct*)

$Al_{11}CeMgO_{19}$ IC-000393

Aluminium cerium magnesium oxide ($Al_{11}CeMgO_{19}$)

[55070-88-7]

$CeMgAl_{11}O_{19}$

M 765.2

Green emitting phosphor for fluorescent lamps. When doped with $Tb^{3\oplus}$.

[57035-62-8]

Verstegen, J.M.P.J. *et al*, *J. Lumin.*, 1974, **9**, 406 (*struct*)
Sommerdijk, J.L. *et al*, *J. Lumin.*, 1976, **14**, 91 (*optical props*)
Ger. Pat., 2 652 472, (1977); *CA*, **87**, 110447 (*use*)
Stevels, A.L.N., *J. Electrochem. Soc.*, 1978, **125**, 588 (*luminescence*)
U.S. Pat., 4 088 922, (1978); *CA*, **89**, 121750 (*use, synth*)

$Al_{11}GaO_{17}$ IC-000394

Aluminium gallium(*I*) oxide ($Al_{11}GaO_{17}$)

Gallium(1) β-alumina

$Al_{11}GaO_{17}$

M 638.5

Red brown air- and moisture-stable cryst. Bleaches at 540°. See Aluminium sodium oxide ($Al_{11}NaO_{17}$), IC-000395.

Radzilowski, R.H., *Inorg. Chem.*, 1969, **8**, 994 (*synth, powder struct*)
Inorg. Synth., 1979, **19**, 51 (*synth*)

$Al_{11}NaO_{17}$ IC-000395

Aluminium sodium oxide ($Al_{11}NaO_{17}$)

β-Alumina

[12005-48-0]

$Na[Al_{11}O_{17}]$

M 591.7

Non-stoichiometric: contains more Na than indicated by ideal formula. Spinel-like layers 1123 pm thick with Na between. Synth. from Na_2CO_3, $NaNO_3$, NaOH and Al_2O_3 at 1500°. Important solid state electrolyte e.g. in Na-S batteries. Commercially available. White cryst. Mp 1950-2000°. Similar compds. with Na replaced by Ag(*I*), Tl(*I*), Li, K, Rb, NH_4, NO, Ga also descr. n_g^D 1.6254 n_o^D 1.6655. Conductivity 3 Ω^{-1} m^{-1}.

Yu Yao, Y.-F. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 2453 (*electrical props, reactions*)
Radzilowski, R.H. *et al*, *Inorg. Chem.*, 1969, **8**, 994, 2531 (*synth, powder struct, ir*)
de Vries, R.C. *et al*, *J. Am. Ceram. Soc.*, 1969, **52**, 364 (*rev*)
Peters, C.R. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 1826 (*cryst struct*)
Radzilowski, R.H. *et al*, *J. Electrochem. Soc.*, 1971, **118**, 714 (*synth*)
Kummer, J.T., *Prog. Solid State Chem.*, 1972, **7**, 141 (*rev*)
Inorg. Synth., 1979, **19**, 51 (*ion exch*)
Müller, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1277 (*Al-27 nmr*)

$Al_{12}CaO_{19}$ IC-000396

Aluminium calcium oxide ($Al_{12}CaO_{19}$)

CA_6

[12005-50-4]

$CaAl_{12}O_{19}$

M 667.8

Structure has 4, 5 and 6-coord. Al. Synth. from oxide melt. Constituent of cement and of steelmaking slags. Refractory and base for rare earth phosphors. White cryst. Mp 1455°.

Nurse, R.W. *et al*, *Trans. Brit. Ceram. Soc.*, 1965, **64**, 409 (*phase diagram*)
Kato, K. *et al*, *Neues Jahrb. Mineral., Abh.*, 1968, **109**, 192 (*cryst struct*)
Imlach, J.A. *et al*, *Trans. Brit. Ceram. Soc.*, 1973, **72**, 221 (*phase diagram, ternary and quaternary systems*)
Chemekova, T.Yu. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, **10**, 2191 (*synth*)
Vyrik, G.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1975, **11**, 1297 (*synth*)
Allibert, M. *et al*, *J. Am. Ceram. Soc.*, 1981, **64**, 307 (*thermodyn data*)
Müller, D., *Polyhedron*, 1986, **5**, 779 (*Al-27 nmr*)

$Al_{12}Na_{12}O_{48}Si_{12}$ IC-000397

Losod

$Na[AlSiO_4].1.5H_2O$

M 1704.6

Zeolite struct. LOS. Member of Chabazite group. Struct. comprises columns of 11 and 17-hedra with apertures formed only by $(Si,Al—O)_6$ connections . Each 11 hedra column is surrounded by 6 17-hedra columns. Synth. from $[N[(CH_2)_4]_2]OH$, $Al(O^iPr)_3$, $Si(OMe)_4$ and aq. MeOH at 100°. Platy hexagonal interpenetrating white cryst. (H_2O).

Sieber, W. *et al*, *Helv. Chim. Acta*, 1974, **57**, 1533 (*synth, props*)
Klinowski, J. *et al*, *J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Fyfe, C.A. *et al*, *J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 82.

$Al_{12}Na_{12}O_{48}Si_{12}$ IC-000398

Zeolite A

Linde Sieve A

M 1704.6

First industrially produced (Linde Corporation) synthetic zeolite. Struct. with 3 D channels and $(Al,Si—O)_8$ rings has β cages of sodalite struct. and α cages with cuboctahedral cavities. Used in various ion exchanged forms, most commonly 3A, 4A, 5A. Ion exchange affects apparent pore radius as exchanged cations fill cavities and may block flow. Activated by dehydrating. Absorbs up to 27 H_2O molecules per unit formula. Zeolite struct. type LTA. One of the Faujasite group. Widely used as a molecular sieve, drying agent, and shape-sensitive cracking catalyst. White cryst. (H_2O).

Na form: Molecular sieve 4A. Zeolite 4A
$Al_{12}Na_{12}O_{48}Si_{12}$ M 1704.6
Main form of zeolite A; starting material for ion exchanged forms. Limiting channel diameter of 410 pm. Ring partially blocked by $Na^{\oplus}$. Ag, Co, Cr, Fe, Mn, Cs, Sr and other ion exchanged forms descr.

K form: Molecular 3A. Zeolite 3A
$Al_{12}K_{12}O_{48}Si_{12}$ M 1897.9
Synth. from Na form by ion exchange.

Ca form: Molecular sieve 5A. Zeolite 5A
$Al_{12}Ca_6O_{48}Si_{12}$ M 1669.2
Synth. from Na form by ion exchange. Permeable to n-hydrocarbons, widely used in hydrocarbon separation.

Breck, D.W. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 5963, 5972 (*cryst struct*)
Barrer, R.M. *et al*, *Trans. Faraday Soc.*, 1958, **54**, 1074 (*ion exch props*)
U.S. Pat., 2 882 244, (1959); *CA*, **53**, 13454 (*synth*)
Howell, P.A., *Acta Crystallogr.*, 1960, **13**, 737 (*cryst struct, Cs form*)
Barrer, R.M. *et al*, *J. Chem. Soc.*, 1961, 971 (*synth*)
Aiello, R. *et al*, *J. Chem. Soc. A*, 1970, 1470 (*synth*)
Kühl, G.H. *et al*, *Inorg. Chem.*, 1971, **10**, 2488 (*synth, props, high silica form*)
Charnell, J.F., *J. Crystal Growth*, 1971, **8**, 291 (*synth*)
Gramlich, V. *et al*, *Z. Kristallogr.*, 1971, **133**, 134 (*cryst struct*)
Yanagida, R.Y. *et al*, *J. Phys. Chem.*, 1973, **77**, 805 (*cryst struct, Ca form*)
Seff, K., *Acc. Chem. Res.*, 1976, **9**, 121 (*use*)
Firor, R.L. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3091 (*cryst struct, Na form*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4992 (*Si-29 nmr*)
Kilnowski, J. *et al*, *J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Fyfe, C.A. *et al*, *J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Inorg. Synth., 1983, **22**, 61 (*synth*)
Pluth, J.J. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 1192 (*cryst struct, Ca form*)
Nagy, J.B. *et al*, *Zeolites*, 1984, **4**, 133 (*Al-27 nmr*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 86.
Tijink, G.A.H. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 7301 (*Na-23 nmr*)
Heo, N.H. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 7986 (*cryst struct, Cs form*)

$Al_{13}ClF_9H_9O_{29}Si_5$ IC-000399

Zunyite

[63957-81-3]

$Al_{13}[Si_5O_{16}](OH,F)_{18}O_4Cl$

M 1170.6

$Al_{13}H_{47}O_{40}^{9\oplus} - Al_{18}B_4O_{33}$

Mineral. Also formulated as $Al_{13}ClF_4(OH)_{14}(SiO_4)_5$. Occurs with variable Si to Al ratios with excess Al replacing Si. A branched oligosilicate. Found in aluminous shales in a variety of locations. Minute, transparent tetrahedra.

[12199-82-5]

Vermaas, F.H.S., *Am. Mineral.*, 1952, **37**, 960 (*occur*)
Baur, W.H. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 390 (*cryst struct*)
Kunwar, A.C. *et al*, *J. Magn. Reson.*, 1984, **60**, 467 (*Al-27 nmr*)
Magi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

IC-000400

$Al_{13}H_{47}O_{40}^{6\oplus}$

Undecaaquatetracosa-μ-hydroxyhydroxytetra-μ_4-oxotridecaaluminium(6+)

$[Al_{13}(OH)_{25}O_4(OH_2)_{11}]^{6\oplus}$

M 1038.1 (ion)

Hexachloride: [78666-02-1]. *Aluminium chloride hydroxide oxide ($Al_{13}Cl_6(OH)_{25}O_4$) undecahydrate*
$Al_{13}Cl_6H_{47}O_{40}$ M 1250.8
Synth. from corresp. sulfate + $BaCl_2$. White solid (aq. Me_2CO 1:25). Sol. H_2O.

Tris-sulfate: [78511-54-3]. *Aluminium hydroxide oxide sulfate ($Al_{13}(OH)_{27}O_4(SO_4)_3$) undecahydrate*
$Al_{13}H_{47}O_{52}S_3$ M 1526.2
Synth. from $AlCl_3$, Na_2SO_4, NaOH. White efflorescent plates (H_2O).

Johansson, G., *Ark. Kemi.*, 1963, **20**, 321 (*cryst struct*)
Müller, D. *et al*, *Chem. Phys. Lett.*, 1981, **79**, 59 (*Al-27 nmr*)
Schönherr, S. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **476**, 188 (*synth, Al-27 nmr, dist*)

IC-000401

$Al_{13}H_{46}O_{56}S_4^{\ominus}$

Dodecaaquatetracosahydroxytetraoxotetrakis [sulfato(2–)]tridecaaluminate(1–)

[12703-68-3]

$[Al_{13}(SO_4)_4O_4(OH)_{24}(OH_2)_{12}]^{\ominus}$

M 1423.3 (ion)

Detected as species in hydrol. of $[Al(OH_2)_6]^{3\oplus}$. Contains twelve edge sharing AlO_6 octahedra round one AlO_4 tetrahedron. Used in synth. of pillared aluminosilicates. Corresponding seleniato species also descr.

Na salt: [62863-58-5].
$Al_{13}H_{46}NaO_{56}S_4$ M 1446.3
White efflorescent cryst. (H_2O).

Johansson, G. *et al*, *Acta Chem. Scand.*, 1960, **14**, 769, 771 (*cryst struct*)
Johansson, G., *Ark. Kemi.*, 1963, **20**, 305 (*selenato species*)
Aveston, J., *J. Chem. Soc.*, 1965, 4459 (*thermodyn data*)
Messner, R.E. *et al*, *Inorg. Chem.*, 1971, **10**, 2290 (*thermodyn data*)
Akitt, J.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 604; 1981, 1608, 1609 (*Al-27 nmr*)
Akitt, J.W. *et al*, *J. Magn. Reson.*, 1978, **32**, 345 (*Al-27 nmr*)
Bottero, J.Y. *et al*, *J. Phys. Chem.*, 1980, **84**, 2933 (*potentiometric titrat*)
Tokarz, M. *et al*, *Clays Clay Miner.*, 1985, **33**, 89 (*use*)
Müller, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1277 (*Al-27 nmr*)
Cheng, S. *et al*, *Inorg. Chem.*, 1989, **28**, 1283 (*synth, use*)
Olivera-Pastor, P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 751 (*use*)

IC-000402

$Al_{14}Ca_{12}O_{33}$

Aluminium calcium oxide ($Al_{14}Ca_{12}O_{33}$)

$C_{12}A_7$

[12005-57-1]

$Ca_{12}[Al_{14}O_{33}]$

M 1386.6

Struct. has AlO_4 tetrahedra which share edges and corners, and 7-coord. Ca. Synth. from molten oxides. White cryst.

Nurse, R.W. *et al*, *Trans. Brit. Ceram. Soc.*, 1965, **64**, 409 (*phase diagram*)
Cockayne, B., *J. Am. Ceram. Soc.*, 1966, **49**, 204 (*synth*)
Oudalov, Y.B. *et al*, *Mater. Res. Bull.*, 1969, **4**, 887 (*synth*)
Bartl, H. *et al*, *Neues Jahrb. Mineral., Monatsh.*, 1969, 404; 1970, 547; *CA*, **71**, 85697; **74**, 104229 (*cryst struct*)
Imlach, J.A. *et al*, *Trans. Brit. Ceram. Soc.*, 1973, **72**, 221 (*syst with FeO*)
Allibert, M. *et al*, *J. Am. Ceram. Soc.*, 1981, **64**, 307 (*thermodyn data*)
Müller, D. *et al*, *Polyhedron*, 1986, **5**, 779 (*Al-27 nmr*)

IC-000403

$Al_{15}Na_{15}O_{96}Si_{33}$

Zeolite ZK-5

$Na_{30}[Al_{30}Si_{16}O_{192}].98H_2O$

M 3212.3

Zeolite struct. KFI has truncated cuboctahedra linked via double $(Al,Si—O)_6$ rings in a body-centred array giving two non-connecting sets of 3 D channels (390 pm across). Member of faujasite group. Synth. from sodium aluminate-silica gels in presence of $[MeN(CH_2CH_2)_3NMe](OH)_2$. Applications similar to those of Linde A. White cryst. (H_2O). Similar aluminosilicates P and Q with Ba_{15} replacing Na_{30} descr.

Kerr, G.T., *Science (Washington, D.C.)*, 1963, **140**, 1412; *Inorg. Chem.*, 1966, **5**, 1539 (*synth, ion exch props*)
Meier, W.M. *et al*, *Z. Kristallogr.*, 1965, **121**, 211 (*cryst struct*)
Barrer, R.M. *et al*, *Z. Kristallogr.*, 1972, **135**, 374 (*P and Q*)
Barrer, R.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1020 (*synth, props*)
Fischer, R.X. *et al*, *Zeolites*, 1986, **6**, 378 (*nd*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 74.

IC-000404

$Al_{16}BaMg_2O_{27}$

Aluminium barium magnesium oxide ($Al_{16}BaMg_2O_{27}$)

[55134-50-4]

$BaMg_2Al_{16}O_{27}$

M 1049.6

Used as a high-energy blue emitting phosphor for fluorescent lamps when $Eu^{2\oplus}$ doped. Additional green emission obtd. when some $Mn^{2\oplus}$ incorporated.

[63774-55-0, 65187-45-3]

Verstegen, J.M.P.J. *et al*, *J. Electrochem. Soc.*, 1974, **121**, 1627.
Verstegen, J.M.P.J. *et al*, *J. Illum. Eng. Soc.*, 1975, **4**, 90.
De Jager-Veenis, A.W. *et al*, *J. Electrochem. Soc.*, 1976, **123**, 1253.
U.S. Pat., 4 161 457, (1979); *CA*, **91**, 100986 (*synth, use*)

IC-000405

$Al_{18}B_4O_{33}$

Aluminium boron oxide ($Al_{18}B_4O_{33}$)

$Al_{18}B_4O_{33}$

M 1056.8

Synth. from B_2O_3 and Al_2O_3 at 1100°. Solid. Thermal expansion 3.5 x 10^{-6}; thermal cond. 3.8 W m^{-1} K^{-1}; dielectric const. 26. $Al_4B_2O_9$ also descr.

Gielisse, P.J.M. *et al*, *Nature (London)*, 1962, **195**, 70 (*phase diagram*)
Ray, S.P., *Amer. Ceram. Soc. Pap.*, 91st meeting, 1989 (*synth, props*)

IC-000406

$Al_{20}Ca_8Na_4O_{80}Si_{20}$

Thomsonite

[12178-50-6]

$Na_4Ca_8[Al_{20}Si_{20}O_{80}].24H_2O$

M 2793.8

Zeolite struct. THO. Member of natrolite group. Interlinked zig-zag chains give struct. with 3 sets of channels (230 × 390, 220 × 400 pm and variable diameter) each with $(Al,Si—O)_8$ rings. Common mineral. Hydrothermal synth. also descr. Fibrous blade-shaped white cryst. Al may be replaced by Ga. Si may be replaced by Ge.

Barrer, R.M. *et al*, *J. Chem. Soc.*, 1959, 195; 1961, 983 (*synth*)
Wirsching, U., *Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4992; 1986, **108**, 1730 (*Si-29, Al-27 nmr*)
Alberti, A. *et al*, *Zeolites*, 1981, **1**, 91 (*cryst struct*)
Gottardi, G. *et al*, *Natural Zeolites*, Springer, 1985, 57 (*props, ir*)
Pluth, J.J. *et al*, *Zeolites*, 1985, **5**, 74 (*nd*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 132.

IC-000407

$Al_{23}N_5O_{27}$

Aluminium nitride oxide ($Al_{23}N_5O_{27}$)

Aluminium oxynitride spinel. ALON

$Al_{23}O_{27}N_5$

M 1122.5

Corresponds to $5AlN.9Al_2O_3$. Synth. from Al_2O_3 – AlN melt. Window material for uv-vis and i.r. spectroscopy. Transparent solid. Resistant to oxidation <1100° in air. Mp 2050°, Mp 2140°. n_D 1.77. Thermal expansion 7 × 10^{-6} K^{-1}.

Long, G. *et al*, *J. Am. Ceram. Soc.*, 1961, **44**, 255 (*phase diagram*)
McCauley, J.W., *J. Am. Ceram. Soc.*, 1978, **61**, 372; 1979, **62**, 476 (*thermal props*)
Harnett, T.M. *et al*, *Ceram. Eng. Sci. Proc.*, 1982, 67 (*use*)

IC-000408

$Al_{88}Na_{88}O_{384}Si_{134}$

Zeolite Y

$Na_2[Al_2Si_3O_{14}]$

M 12805.5

Important synthetic zeolite, siliceous form of Faujasite, IC-000257. Zeolite struct. FAU with Si:Al 1.5-3. Many ion exchanged forms known (Ac, Ca, Ce, Fe, Mg, Mn, NH_4, Ti, Zn etc.). Synth. from aq. $NaAlO_2$, sodium silicate, SiO_2 and NaOH at 20-175°. Catalyst for fluidised bed cracking or hydrocracking. Possesses ion exchange props. Support for wide range of heterogenous catalysts. White cryst. (H_2O).

Costinoble, M.L. *et al*, *J. Chem. Soc., Faraday Trans. 1*, 1976, **72**, 1877 (*powder struct*)
Lippmaa, E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4992; 1986, **108**, 1730 (*Si-29, Al-27 nmr*)
Maxwell, I.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 523 (*Si-29 nmr*)
Fyfe, C.A. *et al*, *J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Engelhardt, G. *et al*, *Zeolites*, 1982, **2**, 59; 1983, **3**, 233, 239 (*Si-29 nmr*)
Inorg. Synth., 1983, **22**, 61 (*synth*)
Freude, D. *et al*, *Zeolites*, 1983, **3**, 171 (*Al-27 nmr*)
Fejes, P. *et al*, *Zeolites*, 1984, **4**, 73 (*ir*)
Nagy, J.B. *et al*, *Zeolites*, 1984, **4**, 135 (*Al-27 nmr*)
Klinowski, J. *et al*, *J. Chem. Soc., Faraday Trans. 1*, 1985, **81**, 3003 (*Si-29, Al-27 nmr*)
Liu, X. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 582; 1990, 13 (*ir, Si-29 nmr*)
Engelhardt, G. *et al*, *High Resolution Solid State NMR of Silicates and Zeolites*, Wiley, 1987 (*Si-29 nmr*)
Dwyer, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 594 (*ir*)
Goyal, R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1990, 1152 (*nd*)

IC-000409

Am

Americium

[7440-35-9]

Am

M 241.0

Atomic No. 95. Ground state electron config. $[Rn]5f^77s^2$. 12 Isotopes known. Discovered in 1944 by Seaborg, James, Morgan and Ghiorso (Chicago). Polymorphic: α-form (double hcp) transforms into β-form (fcc) at 793° and thence into a bcc form at 1050°, stable up to Mp. ^{241}Am is an α emitter with $t_{\frac{1}{2}}$ 433y. ^{243}Am has $t_{\frac{1}{2}}$ 7380y. Produced in kg. amounts of $^{241}Am/^{243}Am$ by neutron irradiation of ^{239}Pu. Metal obt. from (i) AmF_3 + Ba or Li; (ii) AmO_2 + La; (iii) AmF_4 + Ca and (iv) by thermal dec. of Pt_5Am. ^{241}Am used in thickness gauging, density, medical radiographic measurements. Low-energy γ-source (e.g. smoke-detector alarms). Both ^{241}Am, ^{243}Am used as target materials for production of heavier actinides. Soft, silver-white, ductile, malleable metal. Tarnishes slowly in dry air, reacts with steam, acids. Reacts on heating with H_2, O_2, N_2, Hal_2, C, B etc. Forms various alloys. Mp 1176°. Bp 2067° (est.).

▷ Radioactive – very intense α and γ emitter.

Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 859 (*history*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **5**, 5 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1973-1974, A1, A2, 1976, B1.
Transuranium Elements: Products of Modern Alchemy, (Ed. Seaborg, G.T.), Dowden, Hutchinson and Ross Inc., Stroudsburg, 1978.
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **1**, 456; **19**, 629, 682 (*rev, bibl*)
Edelstein, N.M. *et al*, *Americium and Curium Chemistry and Technology*, Reidel, Dortrecht, 1985 (*rev*)
Reavis, J.G. *et al*, *Radiochim. Acta*, 1985, **38**, 135 (*synth*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1988, 1450 (*rev*)
Kimura, T. *et al*, *Radiochim. Acta*, 1986, **39**, 179 (*synth*)
Schulz, W.W. *et al*, *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, 887 (*rev*)
Spirlet, J.C. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1987, **31**, 1 (*rev, bibl*)
Navratil, J. *et al*, *J. Chem. Educ.*, 1990, **67**, 15 (*rev, Am-241*)
Seaborg, G.T. *et al*, *The Elements Beyond Uranium*, Wiley-Interscience, 1990 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 16.

IC-000410

$AmBr_2$

Americium(*II*) bromide ($AmBr_2$)

Americium dibromide

[39705-49-2]

$AmBr_2$

M 400.8
Isostructural with $EuBr_2$. Synth. from Am + $HgBr_2$ at 300°. Black solid.

Baybarz, R.D., *J. Inorg. Nucl. Chem.*, 1973, **35**, 483 (*synth, struct*)

IC-000411

$AmBr_3$
Americium(*III*) bromide ($AmBr_3$)
Americium tribromide
[14933-38-1]

$AmBr_3$

M 480.7
Possesses the $PuBr_3$ struct. White to pale yellow solid (light brown). Sol. H_2O.

Fried, S., *J. Am. Chem. Soc.*, 1951, **73**, 416 (*synth*)
Asprey, L.B. *et al*, *Inorg. Chem.*, 1965, **4**, 985 (*cryst struct*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*synth, struct*)
Pappalardo, R.G. *et al*, *J. Chem. Phys.*, 1969, **51**, 1182 (*uv-vis*)

IC-000412

$AmCl_2$
Americium(*II*) chloride ($AmCl_2$)
Americium dichloride
[16601-54-0]

$AmCl_2$

M 311.9
Possesses the $PbCl_2$ struct. Synth. from Am + $HgCl_2$ at 300°. Black solid.

Baybarz, R.D. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 483 (*synth, struct*)

IC-000413

$AmCl_3$
Americium(*III*) chloride ($AmCl_3$)
Americium trichloride
[13464-46-5]

$AmCl_3$

M 347.4
Possesses the UCl_3 struct. Pink (yellow) solid. Sol. H_2O. Mp 715°. Subl. 850°.

Hexahydrate: Hexaaquadichloroamericium(III)(*1+*) *chloride*
$AmCl_3H_{12}O_6$ M 455.5
Yellow rose cryst. Sol. H_2O.
Contains $AmCl_2(OH_2)_6^{\oplus}$ and $Cl^{\ominus}$ ions.

Fried, S., *J. Am. Chem. Soc.*, 1951, **73**, 416 (*synth*)
Asprey, L.B. *et al*, *Inorg. Chem.*, 1965, **4**, 985 (*cryst struct*)
Pappalardo, R.G., *J. Chem. Phys.*, 1969, **51**, 1182 (*uv-vis*)
Burns, J.H. *et al*, *Acta Crystallogr., Sect. B*, 1970, **26**, 1885 (*synth, cryst struct*)
Burns, J.H. *et al*, *Inorg. Chem.*, 1971, **10**, 147 (*hexahydrate*)

$AmCl_5^{2\ominus}$
Pentachloroamericate(*III*)(2 –) IC-000414

$[AmCl_5]^{2\ominus}$

M 418.3 (ion)
Di-K salt: [108804-42-8]. *Potassium pentachloroamericate*(III). *Americium potassium chloride* (AmK_2Cl_5)
$AmCl_5K_2$ M 496.5
Tan-yellow solid. K_2PrCl_5 struct., with 7-coord. Am.
Di-Rb salt: [108804-44-0]. *Rubidium pentachloroamericate*(III). *Americium rubidium chloride* ($AmRb_2Cl_5$)
$AmCl_5Rb_2$ M 589.2
Tan-yellow solid. K_2PrCl_5 struct.
Di-NH_4 salt: [108804-43-9].
Tan-yellow solid. K_2PrCl_5 struct. Forms $AmCl_3$ on thermal dec. at 300° *in vacuo*.

Schleid, T. *et al*, *J. Less-Common Met.*, 1987, **127**, 183 (*synth, struct*)

IC-000415

$AmCl_6^{3\ominus}$
Hexachloroamericate(*III*)(3 –)
[33613-61-5]

$[AmCl_6]^{3\ominus}$

M 453.7 (ion)
Na, di-Cs salt: [18865-92-4].
Yellow solid. Sol. H_2O. Fcc struct. (Elpasolite). Ir ν_{AmCl} 241 cm^{-1}. Exhibits temp. independent paramagnetism >40K.
Tri-Cs salt: [18898-43-6].
$AmCl_6Cs_3$ M 852.4
Yellow pink cryst.
Tri-Et_4N salt: [23640-58-6].
Yellow solid.
Tris-Ph_3PH salt: [33613-59-1].
Yellow solid.

Ryan, J.L., *Adv. Chem. Ser.*, 1967, **71**, 331.
Bagnall, K.W. *et al*, *J. Chem. Soc. A*, 1968, 133 (*synth*)
Morss, L.R., *Inorg. Chem.*, 1969, **8**, 1433 (*synth, struct*)
Marcus, Y. *et al*, *Isr. J. Chem.*, 1969, **7**, 37; 1970, **8**, 901 (*synth*)
Barbanel, Yu.A. *et al*, *Radiokhimiya*, 1977, **19**, 537; 1979, **21**, 706 (*uv-vis, ir*)
Chudnovskaya, G.P. *et al*, *Radiokhimiya*, 1985, **27**, 545; *Sov. Radiochem.* (*Engl. Transl.*), 1985, **27**, 503 (*struct, uv-vis*)
Soderholm, L. *et al*, *J. Magn. Magn. Mater.*, 1986, **54-57**, 597 (*magnetism*)

IC-000416

AmF_2O_2
Americium(*VI*) fluoride oxide (AmF_2O_2)
Difluorodioxoamericium(VI). *Americium difluoride dioxide*
[20752-67-4]

AmO_2F_2

M 311.0
Has the 8-coord. UO_2F_2 struct. Light brown solid.

Keenan, T.K. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 381 (*synth, struct*)

IC-000417

AmF_3
Americium(*III*) fluoride (AmF_3)
Americium trifluoride
[13708-80-0]

AmF_3

M 298.0
Possesses the LaF_3 struct. Pink solid. Insol. H_2O. Mp ~1393°.

[87345-83-3]

Fried, S., *J. Am. Chem. Soc.*, 1951, **73**, 417 (*synth*)
Westrum, L.E. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 3397 (*synth*)
Carniglia, S.C. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 1451 (*synth, vp*)
Asprey, L.B. *et al*, *Inorg. Chem.*, 1965, **4**, 985 (*cryst struct*)
Burnett, J.L., *J. Inorg. Nucl. Chem.*, 1966, **28**, 2454 (*synth*)
Nave, S.E. *et al*, *Phys. Rev. B: Condens. Matter*, 1983, **28**, 2317 (*magnetism*)

IC-000418

AmF_4
Americium(*IV*) fluoride (AmF_4)
Americium tetrafluoride
[15947-41-8]

AmF_4

M 317.0
Possesses the UF_4 struct. Synth. from AmF_3 + F_2. Tan solid.

Asprey, L.B., *J. Am. Chem. Soc.*, 1954, **76**, 2019 (*synth*)
Asprey, L.B. *et al*, *J. Inorg. Nucl. Chem.*, 1958, **7**, 27 (*synth, struct*)
Chudinov, E.G. *et al*, *Sov. At. Energy* (*Engl. Transl.*), 1970, **28**, 71 (*synth*)
Conner, W.V., *J. Less-Common Met.*, 1971, **25**, 379 (*synth*)
Asprey, L.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 1121 (*synth, struct*)

IC-000419

AmF_6
Americium(*VI*) fluoride (AmF_6)

AmF_6

M 355.0
Not fully characterised. Synth. from KrF_2 + AmF_3 in HF at 40-60°. Volatile dark brown solid. Sol. HF. Ir ν_{Am-F} 604 cm^{-1}.

Drobyshevskii, Iu.V. *et al*, *Radiokhimiya*, 1980, **22**, 591 (*synth*)
Schulz, W.W. *et al*, *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, 914.

IC-000420

[AmH]
Americium hydrides
***Americium hydride* (*AmH_2*)** [13774-24-8]
AmH_2 M 243.0
Exists over a wide composition range. Fluorite struct. Black powder. Isostructural with Pu, Np analogues. ΔH_f –190 kJ mol^{-1}.

***Americium hydride* (*AmH_3*)** [13774-23-7]
Hexagonal. Black powder, stable only at low temps. (<150° at 1 atm. H_2).

[12642-14-7]

Olson, W.M. *et al*, *J. Phys. Chem.*, 1966, **70**, 2934 (*synth, AmH_2,AmH_3*)
Roddy, J.W., *J. Inorg. Nucl. Chem.*, 1973, **35**, 4141 (*synth, AmH_2*)
Shokoji, N., *Phys. Status Solidi B*, 1983, **118**, 811 (*struct, AmH_2*)

IC-000421

AmH_3O_3
Americium(*III*) hydroxide ($Am(OH)_3$)
Americium trihydroxide
[23323-79-7]

$Am(OH)_3$

M 292.0
9-Coord. Am possesses the UCl_3 struct. Amorphous, pink gelatinous solid which forms crystalline rods on ageing. Insol. H_2O. Oxidised to Am(*IV*) analogue by hypochlorite. $K_{sp} \sim 3 \times 10^{-18}$.

[64309-64-4, 103744-97-4]

Penneman, R.A. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **17**, 138 (*synth*)
Milligan, W.O. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 979 (*synth, cryst struct*)
Haire, R.G. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 843 (*synth, cryst struct*)

IC-000422

AmI_2
Americium(*II*) iodide (AmI_2)
Americium diiodide
[38150-40-2]

AmI_2

M 494.8
Isostructural with EuI_2, 7-coord. Am. Synth. from Am and HgI_2 (300°). Black solid. Mp ~700°. $\mu_{eff} = 6.7\mu_B$.

Baybarz, R.D. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 3427 (*synth, struct*)

IC-000423

AmI_3
Americium(*III*) iodide (AmI_3)
Americium triiodide
[13813-47-3]

AmI_3

M 621.7
Exists in two forms. Yellow solid. Sol. H_2O. Mp 950°.

α-form
Orthorhombic. Possesses the BiI_3 struct.

β-form
Hexagonal. Possesses the $PuBr_3$ struct.

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*cryst struct*)
Fried, S. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 416 (*synth*)
Asprey, L.B. *et al*, *Inorg. Chem.*, 1964, **3**, 1137; 1965, **4**, 985 (*synth, cryst struct*)
Pappalardo, R.G. *et al*, *J. Chem. Phys.*, 1969, **51**, 1182 (*uv-vis*)
Haire, R.G. *et al*, *J. Less-Common Met.*, 1983, **93**, 339 (*synth*)

IC-000424

AmN
Americium nitride (AmN)
[12296-96-7]

AmN

M 255.0
Has NaCl struct. Synth. from Am and N_2/H_2. Lustrous black solid.

[60141-78-8]

Akimoto, Y., *J. Inorg. Nucl. Chem.*, 1967, **29**, 2650 (*synth, struct*)
Charvillat, J.P. *et al*, *Radiochem. Radioanal. Lett.*, 1975, **20**, 371.
Kanellakopulos, B. *et al*, *Transplutonium 1975, Proc. Int. Transplutonium Elem. Symp., 4th, 1975*, 1976, 181 (*magnetism*)
Brooks, M.S.S., *J. Magn. Magn. Mater.*, 1982, **29**, 257.
Radchenko, V.M. *et al*, *Radiokhimiya*, 1982, **24**, 173 (*synth*)
Shimbarev, E.V. *et al*, *Radiokhimiya*, 1984, **26**, 643 (*synth, struct*)
The Chemistry of the Actinide Elements, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, 904 (*rev*)

IC-000425

AmO_2
Americium(*IV*) oxide (AmO_2)
[12005-67-3]

AmO_2

M 273.0
Possesses fluorite struct. Synth. by heating many Am compds. in air at 600-800°. First Am compd. reported. Black solid. Sol. mineral acids. There is evidence for non-stoichiometric phases AmO_{2-x}. Possible antiferromagnetic trans. at 8.5K not confirmed by nd.

[23317-46-6, 53754-11-3]

Zachariasen, W.H., *Acta Crystallogr.*, 1949, **2**, 288 (*synth, struct*)
Zachariasen, W.H., *Phys. Rev.*, 1949, **73**, 1104 (*synth*)
Eyring, L. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 1186 (*synth*)

Mueller, M.H. *et al*, *Acta Crystallogr., Sect. A*, 1974, **30**, 667
Karraker, D.G., *J. Chem. Phys.*, 1975, **63**, 3174 (*magnetism*)
Hurtgen, C. *et al*, *Inorg. Nucl. Chem. Lett.*, 1977, **13**, 179 (*synth*)
Veal, B.W. *et al*, *Phys. Rev. B*, 1977, **15**, 2929 (*pe*)
Gubanov, V.A. *et al*, *J. Phys. Chem. Solids*, 1979, **40**, 17 (*theory*)
Boeuf, A. *et al*, *J. Phys. Lett.*, 1979, **40**, 335 (*nd*)
Morss, L.R. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 2059.

IC-000426

[AmS]

Americium sulfides

Various sulfides reported, AmS, Am_2S_3, $AmS_{1.9}$.

***Americium sulfide* (*AmS*)** [32103-93-8]

AmS M 273.1

Has NaCl struct. Formed from Am_2S_3 at 650°.

***Americium sulfide* (Am_2S_3)** [12446-46-7]

Obt. as α(orthorhombic), β and γ(cubic) forms. α-form is isostructural with Ce_2S_3. γ-form has Th_3P_4 struct. β-Form is probably an oxysulfide $Am_{10}S_{14}O$. Black powder. Dec. to AmS *in vacuo* at 650°.

***Americium sulfide* (AmS_2)** [32702-49-1]

AmS_2 M 305.1

Non-stoichiometric with composition approx. $AmS_{1.9}$. Isostructural with PuS_2. Black solid. Stable *in vacuo* to 800°. At 850°, forms α-Am_2S_3.

Zachariasen, W.H. *et al*, *Acta Crystallogr.*, 1949, **2**, 57.
Damien, D. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 291, 685; 1972, **8**, 317.
Damien, D. *et al*, *Radiochem. Radioanal. Lett.*, 1975, **23**, 145.

Am_2O_3 **IC-000427**

Americium(*III*) oxide (Am_2O_3)

[12234-64-7]

Am_2O_3

M 530.1

Trimorphic. Air-sensitive red-brown or tan solid. Sol. mineral acids.

High-temp form

Formed above 800-900°. Possesses hexagonal La_2O_3 type struct. Mp 2205°. ΔH_f –1690 kJ mol^{-1}

Mid-temp form

Formed in the range 460-800° (900°). Possesses monoclinic Sm_2O_3 type struct.

Low-temp form

Possesses bcc α-Mn_2O_3 type struct. Formed up to 460°.

[12330-47-1]

Chikalla, T.D. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 133.
Chikalla, T.D. *et al*, *Colloq. Int. C.N.R.S.*, 1972, **205**, 351; *CA*, **79**, 24345 (*phases*)
Baybarz, R.D. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 4149.
Berndt, U. *et al*, *Inorg. Nucl. Chem. Lett.*, 1974, **10**, 315.
Soderholm, L. *et al*, *J. Nucl. Mater.*, 1985, **130**, 266 (*magnetism*)
Schulz, W.W. *et al*, *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, 909 (*rev*)

$Am_2O_{12}S_3$

Americium(*III*) sulfate ($Am_2(SO_4)_3$) **IC-000428**

$Am_2(SO_4)_3$

M 770.3

Yellow solid. Sol. H_2O. Dec. to AmO_2 on heating in air > 700°.

Pentahydrate: Yellow cryst. Dehydrates > 500° to anhyd. sulfate.

Octahydrate: [38296-89-8].

Air-stable yellow-pink cryst. Contains 8-coord. Am (four H_2O, four sulfate oxygens), geometry intermed. between dodecahedron and antiprism. Some evidence for dodecahydrate. Loses H_2O on heating.

[80714-49-4]

Hall, G.R. *et al*, *J. Inorg. Nucl. Chem.*, 1957, **4**, 137 (*synth*)
Yakovlev, G.N. *et al*, *Zh. Obshch. Khim.*, 1958, **28**, 2624 (*uv-vis*)
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, **C**, 185 (*rev, bibl*)
Burns, J.H. *et al*, *Inorg. Chem.*, 1972, **11**, 2233 (*cryst struct*)
Haire, R.G. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 837 (*synth, reaction*)

Ar **IC-000429**

Argon

[7440-37-1]

Ar

M 39.9

Atomic No. 18. Ground state electron config. [Ne]$3s^23p^6$. Discovered in air in 1894 by Sir W. Ramsey and M.W. Travers. There are 8 isotopes of which 3 are natural. Abundance: 9300 ppm in air (by vol.). Solid state struct. is ccp or hcp (metastable). Obt. by fractionation of liq. air. Used as inert atmosphere, particularly in welding; as gas fill for electric light bulbs, discharge tubes, and lasers. Commercially available. Colourless, odourless, tasteless, monatomic gas. Forms no true chemical compds. Forms clathrates with H_2O and hydroquinone. Forms complex with HBr. Sol. H_2O (33.6 cm^3 kg^{-1} at 20°). Mp –189.4°. Bp –185.9°. Forms clathrate compds. with phenols.

▷ CF2300000.

[14343-01-2]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1927, **7**, 889 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 1, *Suppl. Vol.*, 1970, 16, 133 (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 139 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **12**, 249 (*rev, bibl*)
Andrews, L., *NATO ASI Ser., Ser. B*, 1983, **90**, 153; *CA*, **99**, 30017 (*solid, ir, rev*)
Harris, I.A. *et al*, *Phys. Rev. Lett.*, 1984, **53**, 2390 (*clusters, ms*)
Bernstein, L.S. *et al*, *J. Chem. Phys.*, 1985, **82**, 4802 (*complex*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 1042 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 20.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 294 (*tox*)

As **IC-000430**

Arsenic

[7440-38-2]

As

M 74.9

Atomic No. 33. Ground state electron config. [Ar] $3d^{10}4s^24p^3$. 14 Isotopes have been reported of which only ^{75}As is natural and stable. The element may have been isol. by Albertus Magnus (1193-1280), but compds. known for many centuries previously. Abundance: 1.8 ppm (earth's crust); 0.003 ppm (sea water). Occurs in coal (1-1500 ppm), petroleum (0.001-0.15 ppm), oil shale (→ 50 ppm) and throughout earth's crust (*ca.* 5 ppm). Also occurs widely as the sulfides, and as the oxide, as well as arsenides of many metals. Obt. from flue dusts from smelting of Cu and Pb concentrates, and by

heating arsenides e.g. $FeAs_2$, and sulfides e.g. FeAsS to 700°. Used as alloys with Pb or Cu. Compds. widely used in agriculture as herbicides, wood preservatives, sheep and cattle dips, and also in the glass and electronics industries. More recently, employed in superconductors. Not readily attacked by H_2O, $OH^\ominus$ or non-oxidising acids. Stable in dry air, but surface oxidises in moist air. Dil. HNO_3 → H_3AsO_3; conc. HNO_3 → Arsenic acid, IC-000500. Hot, conc. H_2SO_4 → Arsenic oxide (As_2O_3), IC-000627 and Arsenic oxide (As_4O_6), IC-000665. Fused NaOH → Na_3AsO_3 + H_2. Ignition in air → Arsenic oxide (As_2O_3), IC-000627, Arsenic oxide (As_4O_6), IC-000665, Arsenic oxide (As_2O_5), IC-000630. In vapour, As_4 → As_2 at 800°.

▷ CG0525000.

α-form

Hexagonal lattice. Consists of puckered sheets of covalently bonded atoms of coordn. no. 3 with As—As 251.7 pm, AsAsAs 96.7°, (3 neighbours). As—As 312.0 pm (3 next nearest neighbours). Steel-grey, brittle, stable, 'metallic' form. Mp 816° (38.6 atm.). Subl. 615°. d^{26} 5.78 g cm^{-3}.

Yellow cryst.-form

Cubic lattice containing As_4 molecules. Synth. by sublimation. d^{25} 1.97 g cm^{-3}.

β-form

From As vapour at 200°. Amorphous mirror-like arsenic.

γ-form

From As vapour at 100° or by reduction of H_2O sol. As(*III*) compds. Grey-black amorphous solid but also exists in other colours.

Yellow-form

From As vapour at –100° by rapid quenching. Amorphous plastic. Transforms into the α-form on warming.

Mineral-form

Arsenolamprite, *α-Arsenic*

A semiconducting form. A rare cryst. mineral form.

[23878-46-8, 51680-82-1]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 1 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952 (*rev, bibl*)
Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 91 (*history*)
Calvert, L.D. *et al*, *J. Mater. Sci.*, 1972, **7**, 595 (*cryst struct*)
Duggin, M.J., *J. Phys. Chem. Solids*, 1972, **33**, 1267.
Lucovsky, G. *et al*, *Phys. Rev. B*, 1974, **10**, 4324 (*ir*)
Roberts, E.D. *et al*, *J. Phys. C*, 1975, **8**, 1301 (*pe*)
Smith, P.M. *et al*, *Philos. Mag.*, 1975, **31**, 57 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 567.
Pinto, S.S. *et al*, *Ann. Rev. Pharmacol. Toxicol.*, 1976, **16**, 95 (*haz*)
Moore, L.O., *Encycl. Chem. Process. Des.*, 1977, **3**, 396.
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **3**, 243, 251 (*rev, bibl*)
Petersen, G.L. *et al*, *J. Mol. Struct.*, 1980, **58**, 263 (*nqr*)
Trodahl, H.J. *et al*, *Philos. Mag., Part B*, 1980, **41**, 585 (*ir*)
Takahashi, T. *et al*, *Phys. Rev. B*, 1981, **24**, 3663 (*pe*)
Kidd, R.G., *NATO ASI Ser., Ser. C*, 1983, **103**, 379 (*As-75 nmr*)
Top. Environ. Health, (Ed. Fowler, B.A.), 1983, **6** (*tox, metab, anal*)
Parygin, A.V. *et al*, *Chem. Phys. Lett.*, 1985, **113**, 314 (*nqr*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 637 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 22.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 298 (*tox*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 50 (*haz*)

$AsAuNa_2$ **IC-000431**

Gold sodium arsenide ($AuNa_2As$), 10CI

Disodium arsenidoaurate(2–)

[75228-60-3]

Na_2AuAs

M 317.8

May be regarded as $(Na^\oplus)_2(AuAs)^{2\ominus}$. Struct. comprises zig-zag chains resembling gold(*I*) halides. The gold atoms have linear coordination geometries. Orthorhombic cryst. K_2AuSb is isotypic.

Mues, C. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1055 (*synth, cryst struct*)

[AsB] **IC-000432**

Boron arsenides

Arsenic borides

[51845-78-4]

Boron arsenide* (*BAs*), *9CI, 8CI [12005-69-5]

Arsenic monoboride (*AsB*)

AsB M 85.7

Zinc blende struct. Synth. from BCl_3 and $AsCl_3$ under H_2; or from BBr_3 + As under H_2. Pink acicular cryst. Insol. common acids and alkalis at r.t. or at the boil. Generally chemically inert, but reacts slowly with aqua regia or quickly with boiling HNO_3. Slowly attacked by NaO_2-NaOH at 400°. Vaporises incongr. → As. Semiconductor.

Boron arsenide* (*B_6As*), *9CI, 8CI [12005-70-8]

Arsenic hexaboride (*AsB_6*)

AsB_6 M 139.7

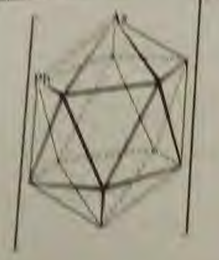
Rhombohedral lattice containing B_6 octahedra with α-B struct. Probably identical to As_2B_{12} and As_2B_{13}. Synth. from B + As at 1000-1200° or BCl_3 + $AsCl_3$ under H_2; Zn_3As_2 + BCl_3 at 600-1000°. Stable to boiling conc. HCl and conc. aq. NaOH. No reaction with boiling conc. HNO_3. Slowly dec. by boiling conc. H_2SO_4.

[56363-92-9]

Williams, F.V. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 1330 (*synth*)
Eliseev, A.A. *et al*, *Zh. Neorg. Khim.*, 1964, **9**, 1158; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 633 (*synth, cryst struct*)
Armington, A.F., *J. Crystal Growth*, 1967, **1**, 47 (*single cryst*)
Krenev, V.A. *et al*, *Zh. Neorg. Khim.*, 1968, **13**, 1279; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 669 (*synth*)
Radchenko, A.F. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 767; 1978, **14**, 1345; *Inorg. Materials* (*Engl. Transl.*), 1972, **8**, 667; 1978, **14**, 1051 (*synth, cryst struct, props*)
Krenev, V.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 1241; *Inorg. Materials* (*Engl. Transl.*), 1972, **8**, 1093 (*synth, props*)
Chu, T.L. *et al*, *J. Electrochem. Soc.*, 1974, **121**, 412 (*synth, props*)
Becher, H.J. *et al*, *Z. Anorg. Allg. Chem.*, 1974, **410**, 274; 1980, **469**, 7 (*ir*)
Alikhanyan, A.S. *et al*, *Zh. Neorg. Khim.*, 1975, **20**, 3090; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 1709 (*synth, ms*)
Bouix, J. *et al*, *J. Crystal Growth*, 1977, **38**, 61 (*synth*)
Hillel, R. *et al*, *J. Crystal Growth*, 1977, **38**, 67 (*synth*)

$AsB_{10}H_{12}Ph^{\ominus}$ IC-000433

1,2-Arsaphenylhadodecaborate(1−)



M 408.3 (ion)
chloro-
Me_4N *salt:* [11093-36-0].
Colourless solid. Sol. MeCN, DMSO; insol. H_2O, hexane.
Hanusa, T.P. *et al., Inorg. Chem.*, 1983, **26**, 4100 (*synth, ir, pmr, B-11 nmr*)

$AsB_{10}H_{10}Sb$ IC-000434

1-Arsa-2-stibadodecaborane(10), 10Cl

(60331-86-8)

M 314.8
closo- Off-white solid. Sol. C_6H_6, DMF. Mp ~300°.
Little, J.L. *et al., Inorg. Chem.*, 1979, **18**, 1598 (*synth, ir, B-11 nmr, mol*)

$AsB_{10}H_{12}^{\ominus}$ IC-000435

Dodecahydro-7-arsenanodecaborate(1−), 10Cl, 9Cl

M 195.1 (ion)
nido-
Me_4N *salt:* [52668-45-8].
Colourless cryst. (H_2O). Sol. MeCN.
Little, J.L. *et al., Inorg. Chem.*, 1974, **7**, 1752 (*synth, ir, pmr, B-11 nmr*)
Hanusa, T.P. *et al., Inorg. Chem.*, 1987, **26**, 4100 (*synth*)

AsBrS IC-000436

Arsenic bromide sulfide (AsBrS), 8Cl

Arsenenethioic bromide, 9Cl

[33369-94-2]

Br—As=S

M 186.8
Vitreous form synth. from mixture of elements; possibly from As_2S_3 + $AsBr_3$. Also $TeBr_4$ + As_2S_3. Mp 70°. Softens at *ca.* 50°.
Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 461 (*rev, bibl*)
Mel'nichenko, F.N. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 1065; *Inorg. Materials (Engl. Transl.)*, 1971, **7**, 945 (*synth, props*)
Slivka, V.Yu. *et al., Fiz. Khim. Stekla*, 1976, **2**, 566; *Sov. J. Glass Phys. Chem. (Engl. Transl.)*, 1976, **2**, 543 (*synth, raman*)

$AsBr_3$ IC-000437

Arsenic bromide ($AsBr_3$)

Arsenous tribromide, 9Cl. Arsenic tribromide. Tribromoarsine. Tribromoarsenic(III)

[7784-33-0]

$AsBr_3$

M 314.6
Pyramidal struct. in vapour phase, interatomic distance: As—Br 233 pm; angle: BrAsBr 99.7°. Synth. from As + Br_2; As_2O_3 + S + Br_2. As_2O_3 or As_2O_5, or sulfides + HBr_3. Commercially available. Colourless, deliquescent rhombic prisms. Fumes in air. Sol. Et_2O, C_6H_6, CS_2, hydrocarbons. Mp 32-33° (31.2°). Bp 221°, Bp_{5} 90°. Hydrol. by H_2O → As_2O_3 + HBr. $\Delta H^{\circ}_{f,298}$ −197 kJ mol^{-1}. Exhibits v. low electrical conductivity when pure
B-CG1375000.

Hexaethylbenzene complex (2:1): [106988-54-9].
$C_{18}H_{30}As_2Br_6$ M 875.7
Rhombohedral cryst. Mp 113°. Only sl. sensitive to air and moisture. Struct. $Br_3As—C_6Et_6—AsBr_3$.

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 392 (*rev, bibl*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1967, 129 (*synth*)
Singh, A.K. *et al., Z. Kristallogr.*, 1967, **124**, 378 (*cryst struct*)
Davies, J.E.D. *et al., J. Chem. Soc. A*, 1968, 1757, 1761; 1971, 1273 (*ir, raman*)
Stufkens, D.J., *Rec. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1970, **89**, 755 (*ir, raman*)
Clark, R.J.H. *et al., J. Mol. Spectrosc.*, 1974, **52**, 58 (*raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 574 (*synth*)
Peel, J.B. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1976, **9**, 175 (*pe*)
Samdal, S. *et al., J. Mol. Struct.*, 1976, **35**, 67 (*ed, struct*)
Robiette, A.G., *J. Mol. Struct.*, 1976, **35**, 81 (*microwave, struct*)
Pabst, R.E. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1980, **33**, 187 (*ms*)
Daly, J. *et al., J. Solid State Chem.*, 1982, **44**, 1 (*cryst struct, rev*)
Grodzicki, M. *et al., Z. Naturforsch., B*, 1984, **39**, 1319 (*pe, struct*)
Schmidbaur, H. *et al., Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 234 (*addnct, ir, cryst struct*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 302 (*haz, tox*)

$AsBr_4^{\ominus}$ IC-000438

Tetrabromoarsenate(*III*)(1−)

[20791-05-3]

$[AsBr_4]^{\ominus}$

M 394.5 (ion)

H compd.: see *Hydrogen tetrabromoarsenate*(III)(1−), *IC-000439*
Tetrabutylammonium salt: [26814-25-5].
Pale yellow solid (CCl_4/$MeNO_2$). Mp 88-90°.
Alijah, G.Y. *et al., J. Chem. Soc. A*, 1970, 326 (*synth, ir, raman, props*)

$AsBr_4H$ IC-000439

Hydrogen tetrabromoarsenate(*III*)(1−), 9Cl, 8Cl

Tetrabromoarsenic(III) *acid*

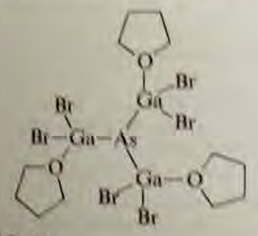
$H[AsBr_4]$

M 395.5
Salts obt. from $AsBr_3$ + amine.HBr in HBr (aq.). Acid is extractable into dibutyl ether.
Me_2NH salt: [66925-73-3].
Yellowish cryst. (Me_2CO/2-propanol). Mp 192-194°.
Dipropylamine salt: [66925-74-4].
Greyish cryst. (Me_2CO/2-propanol). Mp 98-100°.
Tributylamine salt: [66925-77-7].
Greyish cryst. (Me_2CO/2-propanol). Mp 173-175°.
Benzylamine salt: [66925-76-6].
Greyish cryst. (Me_2CO/2-propanol). Mp 128-130°.
Py salt: [93057-71-7].
Pale yellow cryst. Mp 127°. Anion is polymeric based on $AsBr_4^{\ominus}$ chains. Interatomic distances: As—Br 239.5-313 pm; angle: BrAsBr 83.1-96.7°, and 176.3°.
Quinoline salt: [66925-75-5].
Yellowish cryst. (Me_2CO/2-propanol). Mp 157-160° (151°).
N-*Methylaniline salt* (*dimeric*): see *Dihydrogen di-μ-bromohexabromodiarsenate, IC-000584*
Davies, J.E.D. *et al., J. Chem. Soc. A*, 1968, 1761 (*ir, raman*)
Jha, N.K. *et al., J. Indian Chem. Soc.*, 1977, **54**, 944 (*synth*)
Rizvi, S.S.A., *Bull. Soc. Chim. Belg.*, 1984, **93**, 13 (*synth*)
Kaub, J. *et al., Z. Naturforsch., B*, 1984, **39**, 1257 (*synth, cryst struct*)

$AsBr_6Ga_3$ IC-000440

μ_3-Arsenidohexabromotrigallium

Tris(dibromogallium)arsenic



Tris-THF-complex

M 763.5
Obt. as tris-THF complex. Synth. from $(Me_3Si)_3As$ and $GaBr_3$ in toluene.
Tris-THF complex: [113007-06-0].
Tris[dibromo(tetrahydrofuran)gallium]arsenic, μ_3-Arsenidynehexabromotris(tetrahydrofuran)trigallium
$C_{12}H_{24}AsBr_6Ga_3O_3$ M 979.8
Pale yellow cryst. (toluene).
Wells, R.L. *et al., J. Chem. Soc., Chem. Commun.*, 1987, 1823 (*synth, cryst struct*)

$AsCaHO_4$ IC-000441

Calcium arsenate (1:1)

Calcium hydrogen orthoarsenate

[15195-00-3]

$CaHAsO_4$

M 180.0
Synth. from $Ca_3(AsO_4)_2$ + 6*M* H_3AsO_4 aq., or from $CaCO_3$ + H_3AsO_4 aq. V. sol. H_2O. When heated → $Ca_2As_2O_7$.
Monohydrate: [30375-02-1].
Synth. from $CaCO_3$ + H_3AsO_4 aq. Rhombic bipyramidal cryst.
Dihydrate: [30621-29-5].
Synth. from CaO + 6*M* H_3AsO_4 aq., or from $CaCl_2$ + Na_2HAsO_4 aq. Monoclinic cryst.
Trihydrate: [29155-65-5].
Interatomic distances: As—O 164.2-173.4, Ca—O 233.6 (mean) pm; angles: OAsO 105.6-113.8°. Struct. comprises orthorhombic Ca—O octahedra sandwiched between AsO_4 tetrahedra. Resultant layers are connected by zig-zag chains of H bonds.

Mineral-form [24503-14-8]
Weilite
$AsCaHO_4$ M 180.0
The anhydrous salt. Triclinic. Contains two crystallographically independent Ca s coordinated respectively by 7 and 8 O atoms. The AsO_4 tetrahedra are in layers with As—O 166.1-172.2 pm and OAsO 104.0-114.9°. Occurs as secondary mineral at sites in France and Germany. White powder or encrustation.

Mineral-form [14646-95-8]
Haidingerite
$AsCaH_3O_5$ M 198.0
Orthorhombic. Composite layer struct. of distorted AsO_4 tetrahedra connected in parallel by H-bonds. Ca 7-coord. The Ca—O polyhedra are connected (in different directions) by common edges or common vertices. As—O 165.7-172.9 pm. Identical to monohydrate. Occurs as a secondary mineral at sites in USA, Germany and Czechoslovakia. White cryst.

Mineral-form [14635-82-6]
Pharmacolite
$AsCaH_4O_6$ M 216.0
Monoclinic. Ca atoms are coordinated by 6 oxygens in AsO_4 tetrahedra. Water molecules are at layer surface. Layers are joined by H-bonds. Identical to dihydrate. Mineral found at sites in USA, Germany, Czechoslovakia and France. Colourless to greyish cryst.

Guérin, H., *Ann. Chim.*, (11th Ser.), 1941, **16**, 101.
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1957, 376; *Suppl. Vol.* 1-2, 1956, 376; *Suppl. Vol.* 3, 1961, 1231 (*rev, bibl*)
Binas, H., *Z. Anorg. Allg. Chem.*, 1966, **347**, 133 (*cryst struct*)
Ferraris, G. *et al., Acta Crystallogr., Sect. B*, 1969, **25**, 1544; 1970, **26**, 403; 1971, **27**, 349; 1972, **28**, 209 (*ir, cryst structs*)
Brasse, R. *et al., Bull. Soc. Chim. Fr.*, 1970, 2069 (*synth*)
Iyer, V.J. *et al., Z. Naturforsch., B*, 1970, **25**, 1077 (*ir*)
Donnay, J.D.H. *et al., Krist. Tech.*, 1972, **7**, 9, 17 (*cryst struct, rev, bibl*)
Catti, M. *et al., Acta Crystallogr., Sect. B*, 1973, **29**, 90 (*cryst struct*)
Makhmetov, M.Zh. *et al., Zh. Prikl. Khim. (Leningrad)*, 1979, **52**, 2103; *J. Appl. Chem. USSR (Engl. Transl.)*, 1979, **52**, 1985 (*props*)

IC-000442

AsCd$^{\ominus}$

Arsenidocadmate(1−)

[CdAs]$^{\ominus}$

M 187.3 (ion)
Salts do not contain discrete [CdAs]$^{\ominus}$ units.
Li salt: [35788-15-9]. *Cadmium lithium arsenide (CdLiAs)*
AsCdLi M 194.2
Narrow gap semiconductor.
Na salt: [61389-53-5]. *Cadmium sodium arsenide (CdNaAs)*
AsCdNa M 210.3
Cryst. *anti*-$PbCl_2$ type lattice.
K salt: [61389-49-9]. *Cadmium potassium arsenide (CdKAs)*
AsCdK M 226.4
Cryst.
Ca salt (2:1): [62611-33-0]. *Cadmium calcium arsenide (Cd_2CaAs_2)*
As_2CaCd_2 M 414.7
Cryst. Isotypic with $CaAl_2Si_2$.
Ba salt (2:1): [75661-43-7]. *Barium cadmium arsenide ($BaCd_2As_2$)*
As_2BaCd_2 M 511.9
Cryst. Isotypic with $CaAl_2Si_2$.

Schuster, H.U. *et al, Z. Naturforsch., B*, 1972, **27**, 81 (*synth, powder struct, Li salt*)
Kahlert, H. *et al, Z. Naturforsch., B*, 1976, **31**, 1538 (*synth, cryst struct, K salt*)
Klüfers, P. *et al, Z. Naturforsch., B*, 1977, **32**, 353 (*synth, powder struct, Ca salt*)
Klüfers, P. *et al, Z. Naturforsch., B*, 1977, **32**, 753 (*cryst struct, Ca salt*)
Krenkel, B. *et al, Z. Naturforsch., B*, 1979, **34**, 1686 (*cryst struct, synth, Na salt*)
Klüfers, P. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1984, **169**, 135 (*cryst struct, Ba salt*)
Bronsema, K. *et al, Mater. Res. Bull.*, 1988, **23**, 1247 (*synth, powder struct, electrical prop, Li salt*)

IC-000443

[AsCd]

Cadmium arsenides

Cadmium arsenide (Cd_3As_2) [12006-15-4]
As_2Cd_3 M 487.0
Several cryst. forms known. α-Form (r.t.) is body centred tetragonal with T_c As and Cd; β-form (595°) has fluorite-like struct. High pressure forms also known. Synth. from elements. Semiconductor. Grey cryst. Mp 721°.

von Stackelberg, M. *et al, Z. Phys. Chem., Abt. B*, 1935, **28**, 427 (*cryst struct, α-form*)
Gmelin Handbook Inorg. Chem., Syst. No. 33, 1939, 663
Steingrimsen, G.A. *et al, Acta Crystallogr., Sect. B*, 1968, **24**, 1062 (*cryst struct, α-form*)
Pietraszko, A. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 988 (*cryst struct, α-form*)
Banus, M.D. *et al, High Temp. High Pressures*, 1970, **1**, 269 (*powder struct, high pressure form*)
Pietraszko, A. *et al, Phys. Status Solidi A*, 1973, **18**, 723 (*phase trans*)
Dvoraschevskaya, E.P., *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1975, 49 (*ge*)
Pulkina, K.K. *et al, Zh. Neorg. Khim.*, 1975, **20**, 2026 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1047 (*synth*)
Izotov, A.D. *et al, Kristallografiya*, 1978, **23**, 764 (*phase trans*)
Calliess, M.J. *et al, Lect. Notes Phys.*, 1982, **152**, 167 (*ir*)
Singh, M. *et al, Physica B+C (Amsterdam)*, 1983, **117-118**, 441 (*magnetism*)
Nipan, G.D. *et al, Thermochim. Acta*, 1985, **92**, 599 (*thermal anal, powder struct, phase diagram*)
Wrzeska, J. *et al, Phys. Status Solidi B*, 1986, **133**, 57 (*raman*)
Nipan, G.D. *et al, Zh. Fiz. Khim.*, 1986, **60**, 727 (*phase trans*)
Zdanowicz, L. *et al, J. Non-Cryst. Solids*, 1987, **97-98**, 1203 (*optical props*)

IC-000444

$AsCd_2FO_4$

Cadmium arsenate fluoride ($Cd_2(AsO_4)F$)

[12523-03-4]

$Cd_2(AsO_4)F$

M 382.7
Two octahedral Cd environments: both CdO_4F_2. Isotypic with $Cd_2(PO_4)F$ and $Mn_2(PO_4)F$. Cryst. Mp 1100°.

Engel, G., *Z. Anorg. Allg. Chem.*, 1970, **378**, 49 (*synth*)
Engel, G., *J. Less-Common Met.*, 1989, **154**, 367 (*cryst struct*)

IC-000445

$AsClF_4$

Arsenic chloride fluoride ($AsClF_4$)

Chlorotetrafluoroarsorane, 11Cl.
Chlorotetrafluoroarsenic(V). *Arsenic chloride tetrafluoride*

[94649-43-1]

$AsClF_4$

M 186.3
By pyrolysis of Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591. Above −90°, liq. yields Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591. Mp *ca.* −90° (?).

Claus, F. *et al, Z. Anorg. Allg. Chem.*, 1984, **517**, 207 (*synth, ir, raman*)
Minkwitz, R. *et al, Inorg. Chem.*, 1987, **26**, 2730 (*spectra*)

IC-000446

$AsClF_5^{\ominus}$

Chloropentafluoroarsenate(*V*)(1−), 8Cl

[44430-93-5]

$[AsClF_5]^{\ominus}$ (C_{4v})

M 205.3 (ion)
Synth. from $R_4N^{\oplus}[AsF_5OH]^{\ominus}$ + $POCl_3$.
Me_4N salt: [17652-58-3].
Solid. Dec. at 360°.
Et_4N salt: [17950-49-1].
Solid. Dec. at 259°. Stable with respect to F redistribution.
Tetrapropylammonium salt: [17652-59-4].
Solid. Mp 201°.
Tetrabutylammonium salt: [17950-50-4].
Solid. Mp 186°.

Kolditz, L. *et al, Z. Chem.*, 1967, **7**, 157 (*synth*)
Dove, M.F.A. *et al, J. Chem. Soc., Chem. Commun.*, 1984, 1578 (*As-75 nmr, F-19 nmr*)

IC-000447

AsClO

Arsenic chloride oxide (AsClO)

Arsenenous chloride, 9Cl. Chlorooxoarsine

[14525-25-8]

Cl−As=O

M 126.3
Synth. from $AsCl_3$ + As_2O_3; $AsCl_3$ + O_2; $AsCl_3$ + H_2O; Ag + $AsCl_3(g)$ + O_2 at 1200° with matrix isoln. Highly reactive species.

Flögel, P., *Z. Anorg. Allg. Chem.*, 1972, **389**, 188 (*synth*)
Schnöckel, H. *et al, J. Mol. Struct.*, 1983, **102**, 243 (*synth, ir, struct*)
Binnewies, M., *Z. Anorg. Allg. Chem.*, 1983, **505**, 32 (*synth, ms*)

IC-000448

$AsCl_2F_3$

Arsenic chloride fluoride ($AsCl_2F_3$), 8Cl

Dichlorotrifluoroarsorane, 11Cl. Dichlorotrifluoroarsenic(V). *Arsenic dichloride trifluoride*

[14933-43-8]

$AsCl_2F_3$

M 202.8
Has dimeric ionic structure like Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591 in solid state. Synth. by pyrolysis of Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591. Gas which cryst. at 0° or below.

[109278-32-2]

Weidlein, J. *et al, Z. Anorg. Allg. Chem.*, 1965, **337**, 113 (*synth*)
Claus, F. *et al, Z. Anorg. Allg. Chem.*, 1983, **501**, 19; **506**, 178 (*synth, ir, raman ms*)
Minkwitz, R. *et al, Inorg. Chem.*, 1987, **26**, 2730 (*spectra*)
Minkwitz, R. *et al, Z. Anorg. Allg. Chem.*, 1987, **548**, 103 (*synth*)

IC-000449

$AsCl_3$

Arsenic chloride ($AsCl_3$), 9Cl, 8Cl

Arsenous trichloride, 10Cl. Trichloroarsine. Trichloroarsenic(III). *Arsenic butter (obsol.)*

[7784-34-1]

$AsCl_3$

M 181.2
Pyramidal struct., interatomic distance: As−Cl 216.2pm; angle: ClAsCl 98.9°. From As + Cl_2; or As_2O_3 + HCl; or As_2O_3 + S_2Cl_2 + Cl_2. Has been used in halogenation of nucleosides. Commercially available. Colourless, oily liq. freezing to colourless cryst. with pearly sheen. Fumes in air. Sol. SO_2. d_4^{20} 2.162. Mp −16.2° (−19°). Bp 130°. n_D^{20} 1.5980. Forms complexes with aromatic hydrocarbons and many inorganic spp. V.p. 10 mm (25°).

▷ Extremely toxic. CG1750000.

Benzene adduct (2:1): Benzenebis(trichloroarsenic(III)*)*
$C_6H_6As_2Cl_6$ M 440.6
Mp −25.5°.
1,4-Dimethylbenzene adduct (2:1): (1,4-Dimethylbenzene) bis(trichloroarsenic(III)*)*
$C_8H_{10}As_2Cl_6$ M 468.7
Mp −10°.
Ethylbenzene adduct (2:1): Ethylbenzenebis(trichloroarsenic (III)*)*
$C_8H_{10}As_2Cl_2$ M 326.9
Mp −37°.

Biedenkapp, D. *et al, Z. Naturforsch., B*, 1968, **23**, 172 (*arene adducts, nqr*)
Devyatykh, G.G. *et al, Zh. Neorg. Khim.*, 1968, **13**, 2907; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1497 (*ms*)
Konaka, S. *et al, Bull. Chem. Soc. Jpn.*, 1970, **43**, 1693, 3107 (*ed. struct*)
Grechishkin, V.S. *et al, Zh. Fiz. Khim.*, 1970, **44**, 2933; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1970, **44**, 1673 (*Cl, As nqr*)
Clark, R.J.H. *et al, J. Mol. Spectrosc.*, 1974, **52**, 58 (*raman*)
Otozai, K. *et al, Fresenius' Z. Anal. Chem.*, 1975, **274**, 353 (*gc*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 572 (*synth*)
Kober, F., *Z. Chem.*, 1977, **17**, 194 (*ms*)
Cazzoli, G. *et al, J. Mol. Spectrosc.*, 1978, **69**, 71 (*microwave*)
Daly, J. *et al, J. Solid State Chem.*, 1982, **44**, 1 (*cryst struct*)
Lunelli, B. *et al, J. Mol. Spectrosc.*, 1983, **100**, 174 (*ir*)
Grodzicki, M. *et al, Z. Naturforsch., B*, 1984, **39**, 1319 (*pe, struct*)
Diogidze, O.Sh. *et al, Zh. Fiz. Khim.*, 1986, **60**, 1025; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1986, **60**, 615 (*reaction*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 302.

IC-000450

$AsCl_3O$

Arsenic trichloride oxide, 10Cl

Trichlorooxoarsenic(V). *Arsenic*(V) *chloride oxide (AsCl$_3$O). Trichloroarsine oxide*

[60646-36-8]

As(O)Cl_3

M 197.2
Pyramidal struct. with 'true' As=O bond. White cryst. ($CFCl_3$ at −30 to −78°). Dec. slowly at −25°, and rapidly at 0° → Diarsenic tetrachloride trioxide, IC-000592. ΔH_f° −445 kJ mol^{-1}.

Benfield, P.W.S. *et al, J. Chem. Soc., Chem. Commun.*, 1976, 856 (*formn, ir, raman*)
Seppelt, K. *et al, Z. Anorg. Allg. Chem.*, 1978, **439**, 5 (*synth, ir, raman, ms*)

IC-000451

$AsCl_4^{\ominus}$

Tetrachloroarsenate(*III*)(1−), 9Cl, 8Cl

[20791-04-2]

$[AsCl_4]^{\ominus}$

M 216.7 (ion)
In tetraalkylammonium salts, the anion is probably at least dimeric, and may even be polymeric.
Et_4N salt: [26737-92-8].
White solid (CH_2Cl_2/cyclohexane). Mp 76-79°.
Tetrabutylammonium salt: [31235-00-4].
Polymeric anion.
Ph_4P salt (dimeric): see *Di-μ-chlorohexachlorodiarsenate(2−), IC-000596*
H compd. see *Hydrogen tetrachloroarsenate(1−), IC-000454*

Ahlijah, G.Y. *et al, J. Chem. Soc. A*, 1970, 326 (*synth, ir, raman*)
Stufkens, D.J. *et al, Recl. Trav. Chim. Pays-Bas U. R. Neth. Chem. Soc.*, 1970, **89**, 297 (*synth, ir, raman*)

IC-000452

$AsCl_4^{\oplus}$

Tetrachloroarsonium

Tetrachloroarsenic(1+), 9Cl, 8Cl

[29401-03-4]

$[AsCl_4]^{\oplus}$

M 216.7 (ion)
Hexafluoroarsenate: see *Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591*
Hexachloroantimonate: see *Tetrachloroarsenic(1+) hexachloroantimonate(1−), IC-000458*
Tetrachloroaluminate [16142-85-1].
$AlAsCl_8$ M 385.5
Synth. from $AlCl_3$ + $AsCl_3$ + Cl_2. Colourless, hygroscopic cryst. Reacts exothermically with H_2O. On melting, → $AsCl_3$, Cl_2 + $AlCl_3$, but dec. begins at 60°.
Tetrachlorogallate [87144-64-7].
$AsCl_8Ga$ M 428.2
Synth. from $GaCl_3$ + $AsCl_3$ + Cl_2. Colourless, hygroscopic cryst. Mp ≈ 5°. On melting, dec. → $AsCl_3$, Cl_2 + $GaCl_3$.
Hexafluoroantimonate [69005-07-8].
Synth. from $SbCl_4F$ + AsF_3. White solid. Dec. before melting.

Kolditz, L. *et al, Z. Anorg. Allg. Chem.*, 1958, **296**, 188 (*synth*)
DiLorenzo, J.V. *et al, Inorg. Chem.*, 1967, **6**, 766 (*synth, nqr*)
Ballard, J.G. *et al, Can. J. Chem.*, 1978, **56**, 2947 (*synth, raman*)
Demiray, B. *et al, Z. Naturforsch., A*, 1983, **38**, 811 (*raman*)

IC-000453

$AsCl_4F$

Arsenic chloride fluoride ($AsCl_4F$)

Tetrachlorofluoroarsorane, 11Cl. Tetrachlorofluoroarsenic(V). Arsenic tetrachloride fluoride

[87198-15-0]

$AsCl_4F$

M 235.7

Synth. by pyrolysis of Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591. Gas-phase component during sublimation of Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591. Above −100° → Tetrachloroarsenic(1+) hexafluoroarsenate(1−), IC-000591.

Claus, F. *et al, Z. Anorg. Allg. Chem.*, 1983, **501**, 19 (*form, ir, ms*)
Elbel, S. *et al, J. Chem. Res. (S)*, 1986, 294 (*synth, pe, ms*)
Minkwitz, R. *et al, Z. Anorg. Allg. Chem.*, 1986, **534**, 150 (*synth, raman*)
Minkwitz, R. *et al, Inorg. Chem.*, 1987, **26**, 2730 (*spectra*)

$AsCl_4H$ **IC-000454**

Tetrachloroarsenic(III) acid

Hydrogen tetrachloroarsenate(1−), 9Cl, 8Cl

$H[AsCl_4]$

M 217.7

Anion is probably polymeric. Extractable into dibutyl ether.

Py salt: [29961-87-3].
Synth. from $AsCl_3$ + Py.HCl. Needles (aq. HCl). Mp 114°. Polymeric anion.

Quinolinium salt: Synth. from quinoline. HCl + $AsCl_3$. Needles. Mp 130° (123°). Forms dihydrate, Mp 145°.

N-Methylanilium salt (dimeric): see *Dihydrogen di-μ-chlorohexachlorodiarsenate(III)(2−), IC-000597*

Other salts: see *Tetrachloroarsenate(III)(1−), IC-000451*

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 391 (*rev, bibl*)
Davies, J.E.D. *et al, J. Chem. Soc. A*, 1968, 1761 (*ir, raman*)
Devenney, M.J. *et al, J. Chem. Soc. A*, 1970, 1643 (*synth, ir, raman*)

$AsCl_5$ **IC-000455**

Arsenic(V) chloride ($AsCl_5$)

Pentachloroarsorane, 9Cl. Pentachloroarsenic(V). Arsenic pentachloride

[22441-45-8]

$AsCl_5$ (tbp)

M 252.1

Solid obt. at −105°. Too unstable for isolation at much higher temps. Dec. catalysed by HCl. Forms more stable adducts with $SbCl_5$, PCl_5; ΔH_f° −357 kJ mol^{-1}.

PCl_5 complex (1:1): see *Tetrachlorophosphorus(1+) hexachloroarsenate, IC-000457*

$SbCl_5$ complex (1:1): see *Tetrachloroarsenic(1+) hexafluoroantimonate(1−), IC-000458*

Beattie, I.R. *et al, J. Chem. Soc. A*, 1969, 859 (*attempted synth*)
Seppelt, K., *Z. Anorg. Allg. Chem.*, 1977, **434**, 5 (*synth, ms, ir, raman*)
Minkwitz, R. *et al, Inorg. Chem.*, 1987, **26**, 2730 (*struct*)

$AsCl_6^\ominus$ **IC-000456**

Hexachloroarsenate(V)(1−), 9Cl

[35644-16-7]

$[AsCl_6]^\ominus$

M 287.6 (ion)

Et_4N salt: [19235-71-3].
Cryst. (MeCN). Mp 146.5-149° dec.

Tetrachlorophosphonium salt: see *Tetrachlorophosphorus(1+) hexachloroarsenate, IC-000457*

Schmulbach, C.D., *Inorg. Chem.*, 1965, **4**, 1232 (*synth*)
Beattie, I.R. *et al, J. Chem. Soc. A*, 1967, 712 (*ir, raman*)
DiLorenzo, J.V. *et al, J. Phys. Chem.*, 1968, **72**, 761 (*nqr*)
Dove, M.F.A. *et al, J. Chem. Soc., Chem. Commun.*, 1984, 1578 (*nmr*)

$AsCl_{10}P$ **IC-000457**

Tetrachlorophosphorus(1+) hexachloroarsenate, 9Cl

Tetrachlorophosphonium hexachloroarsenate

[17731-57-6]

$[PCl_4][AsCl_6]$

M 460.4

Synth. from PCl_5 + $AsCl_3$ + Cl_2 in sealed tube at 60°. V. hygroscopic yellow-orange cryst.

Beattie, I.R. *et al, J. Chem. Soc. A*, 1967, 712 (*ir, raman*)
Wicker, W. *et al, Z. Naturforsch., B*, 1967, **22**, 983 (*P-31 nmr*)
Brinkmann, F.J. *et al, Rev. Chim. Minér.*, 1970, **7**, 729 (*synth, raman*)
Demiray, A.F. *et al, Monatsh. Chem.*, 1979, **110**, 799 (*synth, raman*)

$AsCl_{10}Sb$ **IC-000458**

Tetrachloroarsenic(1+) hexachloroantimonate(1−), 9Cl, 8Cl

Tetrachloroarsonium hexachloroantimonate

[24804-94-2]

$[Cl_4As]^\oplus[SbCl_6]^\ominus$

M 551.1

Orthorhombic. Tetrahedral cation weakly associated with octahedral anion. Synth. from $SbCl_5$ + $AsCl_3$ + Cl_2. Pale yellow, hygroscopic cryst., only stable under Cl_2. Can be sublimed by dec. and recombination.

$AsCl_3$ complex: [19453-04-4].
$As_2Cl_{11}Sb$ M 732.4
Orthorhombic, greenish cryst. $AsCl_3$ may be removed *in vacuo*.

[69005-07-8]

Beattie, I.R. *et al, J. Chem. Soc. A*, 1967, 712 (*synth, ir, raman*)
Webster, M. *et al, J. Chem. Soc. A*, 1968, 2166 (*adduct, ir, raman*)
Brinkmann, F.J.J. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1969, **88**, 1358 (*synth, raman*)
Preiss, H., *Z. Anorg. Allg. Chem.*, 1971, **380**, 71; 1972, **389**, 280 (*adduct, cryst struct, ms*)
Ballard, J.G. *et al, Can. J. Chem.*, 1978, **56**, 2947 (*synth, raman*)
Demiray, A.F. *et al, Monatsh. Chem.*, 1979, **110**, 799 (*synth, raman*)

[AsCo] **IC-000459**

Cobalt arsenides

Two phases descr. here.

Cobalt arsenide* ($CoAs_2$), *8Cl [12044-42-7]

Cobalt diarsenide

As_2Co M 208.7

Isotypic with $CoSb_2$. The mineral Smaltite, is an As deficient variety of Skutterudite.

***Cobalt arsenide* ($CoAs_3$)**

Skutterudite

As_3Co M 283.6

Struct. contains well-defined As_4 planar rings disposed in a manner related to ReO_3. The natural mineral contains Ni and is formulated (Co,Ni)As_3. Occurs in medium to high-temp. hydrothermal veins. White metallic cryst.

Kjekshus, A., *Acta Chem. Scand.*, 1971, **25**, 411 (*$CoAs_2$, synth, struct, magnetism*)
Wells, A.F., *Structural Inorg. Chem.*, 5th Edn., O.U.P., 1984, 267 (*$CoAs_3$, struct*)

$AsCoH_{15}N_5O_4$ **IC-000460**

Arsenatopentaamminecobalt(III), 8Cl

[32356-19-7]

$Co(NH_3)_5AsO_4$

M 283.0

Red cryst. solid + $5H_2O$. Phosphate analogue known.

Beech, T.A. *et al, Aust. J. Chem.*, 1971, **24**, 1065; 1973, **26**, 1877 (*synth, ir, raman*)

[AsCr] **IC-000461**

Chromium arsenides

Chromium arsenide* (Cr_2As), *9Cl [12254-85-2]

$AsCr_2$ M 178.9

Has the Cu_2Sb-type struct. A high-temp. Fe_2P-type phase is known. A phase in the Cr-As system. Antiferromagnetic, T_N 393K.

Chromium arsenide* (Cr_3As_2), *9Cl [12255-59-3]

As_2Cr_3 M 305.8

Phase in the Cr-As system. Ferromagnetic with a Curie point of −16°.

Chromium arsenide* ($CrAs$), *9Cl [12044-08-5]

AsCr M 126.9

Adopts a helimagnetic struct. below ~260K. Undergoes a phase transition at 1170K from the MnP to the NiAs struct. type. Phase in the Cr-As system. Grey solid. Insol. H_2O, EtOH.

Nowotny, H. *et al, Z. Phys. Chem., Abt. B*, 1938, **38**, 461 (*synth, cryst struct, Cr_2As*)
Hollan, L. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **260**, 2233 (*synth, magnetism, Cr_3As_2*)
Takeshi, S. *et al, J. Phys. Soc. Jpn.*, 1966, **21**, 2076 (*nmr, Cr_3As_2*)
Wolfsgruber, H. *et al, Monatsh. Chem.*, 1968, **99**, 1230 (*cryst struct, Cr_2As*)
Selte, K. *et al, Acta Chem. Scand.*, 1971, **25**, 1703; 1973, **27**, 3195 (*synth, cryst struct, magnetism, CrAs*)
Yamaguchi, Y. *et al, J. Phys. Soc. Jpn.*, 1972, **32**, 958 (*magnetism, Cr_2As*)
Kallel, A. *et al, J. Phys. Chem. Solids*, 1974, **35**, 1139 (*magnetism, CrAs*)
Blachnik, R. *et al, J. Chem. Thermodyn.*, 1978, **10**, 507 (*thermodynamics, CrAs*)

$AsCuPbS_3$ **IC-000462**

Copper lead arsenide sulfide ($CuPbAsS_3$)

Seligmannite

$PbCuAsS_3$

M 441.8

CuS_4 tetrahedra and AsS_3 pyramids with Pb in large voids. Similar to wurtzite. Mineral found in Tuscany, Italy. Cryst.

Takeuch, Y. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1969, **130**, 254
Edenharter, A. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1970, **131**, 397 (*cryst struct*)

$AsCu_3S_3$ **IC-000463**

Copper arsenic sulfide (Cu_3AsS_3)

Tricopper(1+) thioarsenite, 8Cl. Tricopper(I) arsenic trisulfide

[15117-93-8]

Cu_3AsS_3

M 361.7

Cubic lattice with wurtzite type struct. Defect. struct. with vacancies at ¼ of the S sites. Synth. from the elements. Mp 640°. Struct. stable at high pressure.

Storm, A.R. *et al, J. Phys. Chem. Solids*, 1968, **29**, 623 (*struct*)

$AsCu_3S_4$ **IC-000464**

Tricopper(1+) thioarsenate, 8Cl

Tricopper(1+) arsenotetrathioate, 9Cl. Copper arsenic sulfide (Cu_3AsS_4)

[15117-94-9]

Cu_3AsS_4

M 393.8

Orthorhombic. Dark, purplish grey, granular cryst. Exhibits moderate bireflectance (pale yellowish pink to pinkish grey with violet tint). Distinct anisotropism changing col. from dark blue to reddish orange. Mp 655°.

Mineral-form [14933-50-7]

Enargite

Possesses the wurtzite-type struct. Orthorhombic. Cu—S 230-238 pm, As—S 216-219 pm. Occurs in ores distributed world-wide. Dark grey grains with metallic lustre. Exhibits strong bireflectance (pale pinkish yellow to pale pinkish grey) with strong anisotropism (interference col. dark blue → orange). Obt. from luzonite at 450°.

Mineral-form [12173-86-3]

Luzonite

Possesses zinc blende struct. with As—S 226.5, Cu—S 230.4-233.7 pm. Occurs world-wide. Synth. from CuS + As_2S_3 at 250-350°. Tetragonal deep pinkish brown cryst. with greyish tinge. Stable to 450° when converted into enargite.

Gmelin Handbook Inorg. Chem., Syst. No. 60, *Suppl. Vol.*, 1961, **2**, 960 (*rev, bibl*)
Marumo, F., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1967, **124**, 1 (*cryst struct*)
Storm, A.R. *et al, J. Phys. Chem. Solids*, 1968, **29**, 623
Adiwidjaja, G. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 1879 (*cryst struct*)
Samanta, L.K. *et al, Phys. Status Solidi A*, 1977, **41**, 331 (*optical props*)
Nakai, I. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 789 (*pe*)
Sugaki, A. *et al, Sci. Rep. Res. Inst. Tohoku Univ., Ser. A, Ser. 1*, 1982, **15**, 257 (*synth, props, bibl*)

$AsDyO_4$ **IC-000465**

Dysprosium arsenate ($DyAsO_4$)

[27746-50-5]

$DyAsO_4$

M 301.4

Tetragonal. By reaction between $DyCl_3$ and Na_3AsO_4. Solid. Semiconductor. Ferroelectric. Thermally stable at < 1000°.

Gimbel, H. *et al. Phys. Status Solidi B*, 1972, **50**, 147 (*cryst struct*)
Arapkovich, L.E. *et al. Zh. Neorg. Khim.*, 1973, **18**, 1706, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 901 (*props*)
Lang, F.G. *et al. Can. J. Phys.*, 1977, **55**, 1633 (*cryst struct*)
Smith, S.H. *et al. J. Mater. Sci.*, 1978, **13**, 620 (*synth*)
Gabelkoten, Ts.D. *et al. Ca*, 1980, **93**, 18226 (*synth*)
Donnadieu, G. *et al. J. Magn. Magn. Mater.*, 1980, **15-18**, 37 (*phase, phys props*)

IC-000466

AsF_3

Arsenic fluoride (AsF_3), 8Cl

Arsenous trifluoride, 9Cl. *Trifluoroarsine*. *Trifluoroarsenic*(III)

[7784-33-2]

AsF_3

M 131.9

Detected in Jupiter's atm. Pyramidal struct in gas phase. Interatomic distance As—F 170.6 pm; angle FAsF ~102°. Orthorhombic cryst. system containing distorted tricapped trigonal prisms of F around As. Synth. from As_2O_3 + HF or HSO_3F. Fluorinating agent, although weaker than SbF_5. Commercially available. V. mobile, colourless liq. which fumes in air and readily hydrol. Sol. alcohols, Et_2O, C_6H_6. d^{15} 2.73. Mp −6.0° (−8.5°). Bp 63°. Attacks glass, but not polythene. ΔH_f° −956.5 kJ mol⁻¹; ΔH_f° (g) −910 kJ mol⁻¹.

▷ Very poisonous. CG5775000.

Rivière de Massilioux, O., *J. Mol. Struct.*, 1968, **1**, 203 (*ir*)
Kaneko, K. *et al. Bull. Chem. Soc. Jpn.*, 1970, **43**, 1693 (*ir*)
Clippard, F.B. *et al. Inorg. Chem.*, 1970, **9**, 805 (*ed, struct*)
Rousseau, Y. *et al. Spectrochim. Acta, Part A*, 1970, **26**, 379 (*ir*)
Chivikovskii, Y. *et al. Bull. Chem. Soc. Jpn.*, 1977, **46**, 2314 (*thermochem*)
Clark, R.J.H. *et al. J. Mol. Spectrosc.*, 1976, **62**, 58 (*raman*)
Kazakov, F.K. *et al. Mol. Phys.*, 1975, **29**, 1485 (*F-19 nmr, mpt*)
Brauer, G. *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 213 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 682 (*rev*)
Salzsieder, W.R. *et al. J. Chem. Phys.*, 1979, **71**, 2044 (*ir*)
Unly, I. *et al. J. Solid State Chem.*, 1982, **44**, 3 (*cryst struct*)
Christakis, M. *et al. Z. Kristallogr. – B*, 1984, **39**, 1319 (*pe, struct*)
Sax, N.I. *et al. Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 215

AsF_3O

IC-000467

Arsenic trifluoride, 10Cl

Trifluoroarsine oxide, *Trifluoroarsoarsenic*(V). *Arsenic*(V) *fluoride oxide* (AsF_3O)

[15120-14-6]

$As(O)F_3$

M 147.9

Descr. as a polymer when synth. from AsF_5. Synth. either from glassy As_2O_3 + F_2 or from AsF_5 + Cl_2O. One of few compds. possessing As=O bond. Fumes in air and exotherms with H_2O. Mp −68.3°. Bp −25.6°. ΔH_f° (g) −1011 kJ mol⁻¹.

Mitra, G. *J. Am. Chem. Soc.*, 1938, **80**, 5619 (*synth*)
Seppelt, L. *et al. Z. Anorg. Allg. Chem.*, 1978, **439**, 5 (*attempted synth*)
Downs, A.J. *et al. Inorg. Chem.*, 1982, **21**, 3385 (*synth, ir, struct*)

AsF_4K

Potassium tetrafluoroarsenate(*III*), 9Cl

Potassium fluoroarsenite

[28174-28-9]

$KAsF_4$

M 190.0

Synth. via KAs_2F_7 (at 100°). V. hygroscopic cryst. (AsF_3).

AsF_3 complex: *Potassium heptafluorodiarsenate*

As_3F_7K M 321.9

Synth. from KF + AsF_3. Dec. at 100°. Monoclinic. Chains formed of molecular AsF_3 + tbp AsF_4 anions (lone pair equatorial). Interatomic distances: As—F ($AsF_4^\ominus$) 190.5 (ax.), 174 (eq.) (AsF_3) 171-175, As—F ($AsF_4^\ominus$) 190.5 (ax.), 174 (eq.) (AsF_3) 171-175, As—F 92°, $F_{eq}AsF_{eq}$ 95°, $F_{ax}AsF_{ax}$ 167°. pm; angles: FAF 92°, $F_{eq}AsF_{eq}$ 95°, $F_{ax}AsF_{ax}$ 167°.

Woolf, A.A. *et al, J. Chem. Soc.*, 1950, 2200 (*synth*)
Muetterties, E.L. *et al, J. Am. Chem. Soc.*, 1957, **79**, 3686 (*synth*)
Edwards, E.J. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1630 (*synth, cryst struct*)

AsF_4Tl

IC-000469

Thallium(*I*) tetrafluoroarsenate

$Tl[AsF_4]$

M 355.2

Synth. from excess AsF_3 + TlF in pressure vessel at 80°. Cryst. (AsF_3); v. hygroscopic, rapidly hydrol. by H_2O. Largely dissociated in fused state.

▷ Toxic.

Muetterties, E.L., *J. Am. Chem. Soc.*, 1957, **79**, 3686 (*synth, F-19 nmr, prop*)

AsF_5

IC-000470

Arsenic fluoride (AsF_5), 8Cl

Pentafluoroarsorane, 9Cl. *Pentafluoroarsenic*(V). *Arsenic*(V) *pentafluoride*

[7784-36-3]

AsF_5

M 169.9

Monomeric in vapour. Strong Lewis acid. Tbp struct. with As—F (ax.) 171.1, As—F (eq.) 165.6pm (gas). In the solid, the interatomic distances are 171.9 and 166.8 pm. Synth. from As or As_2O_3 + F_2. Catalyst for dimerisation of propene, and for polymerisation of acetaldehyde and other organics. Complexes with a multitude of substances eg. halogens and interhalogens, nitrogen halides, halides of elements in Groups Vb and VIb. Colourless gas. Hydrol. by H_2O. Sol. EtOH, Et_2O, C_6H_6. d_4^{63} 2.33 (l). Mp −79.8°. Bp −52.9°. Soln. in HF contains AsF_3, $AsF_6^\ominus$ and $As_3F_{11}^\ominus$. ΔH_f° −1238 kJ mol⁻¹.

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 365 (*rev, bibl*)
Jones, E.D. *et al, J. Chem. Phys.*, 1962, **36**, 1691 (*As-75 nmr*)
Hoskins, L.C. *et al, J. Chem. Phys.*, 1967, **46**, 2402 (*ir, raman*)
Clippard, F.B. *et al, Inorg. Chem.*, 1970, **9**, 805 (*ed, struct*)
Brickmann, J., *Ber. Bunsenges. Phys. Chem.*, 1971, **75**, 747 (*struct*)
Vasile, M.J. *et al, Inorg. Chem.*, 1972, **11**, 2282 (*ms*)
Falconer, W.E. *et al, J. Fluorine Chem.*, 1974, **4**, 213 (*ms, struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 216 (*synth*)
Barraclough, C.G. *et al, J. Fluorine Chem.*, 1988, **38**, 405 (*props, raman*)
Ebel, S. *et al, J. Mol. Struct.*, 1988, **175**, 441 (*pe*)
Koehler, J. *et al, Z. Anorg. Allg. Chem.*, 1989, **575**, 55 (*cryst struct*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 51 (*haz*)

$AsF_6^\ominus$

IC-000471

Hexafluoroarsenate(1 −), 9Cl, 8Cl

[16973-45-8]

$[AsF_6]^\ominus$ (O_h)

M 188.9 (ion)

Tetrabutylammonium salt: White needles (MeOH). Mp 245-248°.

K salt: see *Potassium hexafluoroarsenate*(V). *IC-000473*

Bougon, R. *et al, Inorg. Chem.*, 1974, **13**, 690 (*ir*)
Nefedov, V.I. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1975, **6**, 221 (*pe*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 682 (*rev*)
Dove, M.F.A. *et al, J. Chem. Soc., Chem. Commun.*, 1984, 1578 (*F-19 nmr, As-75 nmr*)
Inorg. Synth., 1986, **24**, 138 (*synth*)
Heyns, A.M., *S. Afr. J. Chem.*, 1988, **41**, 97 (*raman*)

AsF_6H

IC-000472

Hexafluoroarsenic acid

Hydrogen hexafluoroarsenate(V), 9Cl, 8Cl

[17068-85-8]

$H[AsF_6]$

M 189.9

Pentahydrate, hydrofluoride: [77152-86-4].
Commercially available acid. Whitish cryst. Mp 25-30°. Probably cubic lattice. Clathrate-like hydrate in which $AsF_6^\ominus$ ions occupy tetradecahedral cages in fully H-bonded lattice. H_2O, $H_3O^\oplus$ and HF randomly distributed.

Hexahydrate: [121995-33-3].
Synth. from $KAsF_6$ in aq. soln. by ion exchange, and evap. Commercially available acid. Hexagonal lattice. Polyhedral clathrate hydrate. $AsF_6^\ominus$ ions occupy the smallest polyhedra.

Difluoromethylamine salt: [42039-54-3].
CH_4AsF_8N M 256.9
Synth. from HCN + AsF_5 in HF(l).

Bis(trifluoromethyl)amine salt:
$C_2H_2AsF_{12}N$ M 342.9
Synth. from $(F_3C)_2NH$ + AsF_5 in HF. Colourless cryst. solid. Stable at r.t. for prolonged periods. V.p. *ca.* 20mm at 22°.

Atkinson, G. *et al, J. Phys. Chem.*, 1960, **64**, 1487 (*synth*)
Lawless, E.W. *et al, Inorg. Chem.*, 1971, **10**, 1084 (*synth*)
Gillespie, R.J. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1261 (*deriv, ir*)
Moreno-Gonzalez, E. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1977, **74**, 563; 1980, **77**, 149 (*deriv, ir*)
Davidson, D.W. *et al, Inorg. Chem.*, 1981, **20**, 2013 (*cryst struct*)
Desmarteau, D.D. *et al, J. Fluorine Chem.*, 1984, **25**, 387 (*salts, raman, F-19 nmr*)
Wiebcke, M. *et al, Z. Kristallogr.*, 1986, **177**, 291; 1988, **183**, 1 (*cryst struct*)
Gantar, D. *et al, Thermochim. Acta*, 1989, **142**, 49 (*ir, raman*)

AsF_6K

IC-000473

Potassium hexafluoroarsenate(*V*), 9Cl

Hexafluoroarsenate(1 −), *potassium salt*, 8Cl

[17029-22-0]

$K[AsF_6]$

M 228.0

Trigonal. As at centre of discrete octahedral anion: As—F 172, K—F 289 pm. Synth. by reaction of a mixt. of a potassium halide and excess arsenicus oxide with HrF. Commercially available. Herbicide. Thick, colourless plates. Melts at red heat with part. dec. Forms a hemihydrate.

▷ Highly toxic, cancer suspect agent. TT1225000.

Rhombohedral-form
Distorted CsCl type. At 101.5° transformed into cubic form.

Cubic-form
Highly distorted anion.

Woolf, A.A. *et al, J. Chem. Soc.*, 1950, 1050 (*synth*)
Roolf, R.B., *Acta Crystallogr.*, 1955, **8**, 779 (*cryst struct*)
Kemmitt, R.D.W. *et al, J. Chem. Soc.*, 1963, 4408 (*cryst struct*)
Haase, D.J. *et al, Chem. Zvesti*, 1965, **19**, 167 (*cryst struct*)
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, 196 (*synth*)
Heyns, A.M. *et al, Spectrochim. Acta, Part A*, 1975, **31**, 1293 (*ir, raman, polymorphs*)
Gabuda, S.P. *et al, Koord. Khim.*, 1979, **5**, 850 (*F-19, As-75 nmr*)
Guo, Q.Z. *et al, J. Magn. Reson.*, 1984, **57**, 136 (*F-19 nmr*)
Heyns, A.M., *S. Afr. J. Chem.*, 1988, **41**, 97 (*raman*)

AsF_6Li

IC-000474

Lithium hexafluoroarsenate(*V*)

Hexafluoroarsenate(1 −) *lithium salt*, 8Cl

[29935-35-1]

$LiAsF_6$

M 195.8

Commercially available. High purity $LiAsF_6$ is prepd. by a metathetical reaction between $KAsF_6$ and $LiClO_4$ in an inert org. solv. such as HCOOMe. Alternative preparation involves reaction of aq. $HAsF_6$ with aq. LiOH. Electrolyte component for lithium battery systems. Rhombohedral white cryst.

▷ Highly toxic cancer suspect agent.

Kemmitt, R.D.W. *et al, J. Chem. Soc.*, 1963, 4408 (*cryst struct*)
U.S. Pat., 3 848 063, (1974); *CA*, 1975, **82**, 43944 (*synth*)
U.S. Pat., 3 907 977, (1975); *CA*, 1976, **84**, 5178 (*synth*)
U.S. Pat., 4 065 550, (1977); *CA*, 1978, **88**, 76049 (*synth*)
Guo, Q.Z. *et al, J. Magn. Reson.*, 1984, **57**, 143 (*F-19 nmr*)

$AsF_6N_3O_6S_3$

IC-000475

Arsinidynetris(imidosulfuryl fluoride), 9Cl

Arsylidynetris(imidosulfuryl fluoride), 8Cl

[33416-68-1]

$As(NSOF_2)_3$

M 375.1

Synth. from $Hg(NSOF_2)_2$ + $AsCl_3$. Liq. Mp −3°. $Bp_{0.3}$ 38°.

Sundermeyer, W. *et al, Angew. Chem., Int. Ed. Engl.*, 1971, **10**, 459 (*synth, ir, F-19 nmr*)
Ilckh, C. *et al, Chem. Ber.*, 1975, **108**, 2580 (*synth, ms, F-19 nmr*)

AsF_6Na

IC-000476

Sodium hexafluoroarsenate(*V*)

Hexafluoroarsenate, sodium salt, 8Cl

[12005-86-6]

$NaAsF_6$

M 211.9

Isostructural with $LiSbF_6$. Synth. either by reaction of BrF_3 on a mixture of NaF and AsO_3 or by fluorination using ClF_3 of As in anhydrous liq. HF followed by reaction with NaF. Commercially available. Colourless rhombohedral cryst.

▷ WB2775000.

Clifford, A.F. et al, J. Inorg. Nucl. Chem., 1957, 5, 71 (synth)
Kemmitt, R.D.W. et al, J. Chem. Soc., 1963, 4408 (struct, synth)
Kolditz, L. et al, Z. Chem., 1963, 3, 312 (ir)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, 4, 1702 (rev, bibl)
Guo, Q.Z. et al, J. Mater. Resea., 1994, 57, 136 (F-19 nmr)

IC-000477

AsF_6Tl

Thallium(*I*) hexafluoroarsenate

$Tl[AsF_6]$

M 393.2

Rhombohedral $KOsF_5$ struct. (distorted CsCl). Synth. from AsF_5 and TlF soln. in SeF_4, excess SeF_4 removed by heating.

▷ Toxic.

Kemmitt, R.D.W. et al, J. Chem. Soc., 1963, 4408 (synth, struct)
Wells, A.F., Structural Inorg. Chem., 5th Ed. Clarendon Press, Oxford, 1984, 457 (struct)

IC-000478

AsFe

Iron arsenide (FeAs)

[12044-16-5]

FeAs

M 130.7

Struct. similar to NiAs. Obt. from direct combination of elements or from H_2 + $FeAs_2$ at 680°. Semiconductor. Component of mineral Modderite, (Co,Fe)As. White. Sl. sol. H_2O. Mp 1020°. Paramagnetic; magnetic ordering occurs at low temp. (5K).

Selte, K. et al, Acta Chem. Scand., 1972, 26, 3101; 1973, 27, 1442 (struct, magnetism)
Yasui, M. et al, J. Phys. Soc. Jpn., 1980, 48, 1937 (antiferromagnetism)
Lomax, P.S. et al, Acta Crystallogr., Sect. B, 1984, 40, 14 (cryst struct)

IC-000479

$AsFeO_3$

Ferric arsenite

Iron(III) arsenite (FeAsO₃)

$FeAsO_3$

M 179.7

Tetrahydrate: [61095-38-1].

Basic salt: Basic iron(III) arsenite. Basic iron(III) orthoarsenite

$As_2Fe_4H_8O_{16}$ M 607.3

Brown-yellow powder. Sol. acid, alkali; insol. H_2O. Formulated as $2FeAsO_3.Fe_2O_3.5H_2O$. Composition may vary. Dec. at Mp.

Gmelin Handbook Inorg. Chem., Syst. No. 58, 1931, B4, 780 (rev, bibl)

$AsFeO_4$

IC-000480

Iron(*III*) arsenate ($FeAsO_4$)

Ferric arsenate. Iron(III) orthoarsenate. Arsenic acid, iron(3+) salt (1:1), 11Cl

[10102-49-5]

$Fe(AsO_4)$

M 194.7

Originally proposed that Fe(*III*) was octahedrally coordinated. Now known to be isostructural with $LiAlH_4$ with 5-coord. Fe. Hydrated salt used for most applications. Synth. from As_2O_5 + $Fe(NO_3)_3.9H_2O$ or $Fe(OH)_3$ in hydrothermal conditions. Component in electrochromic devices. Used to remove As from H_2O.

▷ NO4585000.

Dihydrate: [16103-66-5]. ***Scorodite***

Mineral, occurs widely throughout US and elsewhere. Insecticide. Green-brown powder or large blue cryst. Insol. H_2O; sol. dil. HCl; insol. HNO_3. Dec. on heating.

▷ Toxic by ingestion or inhalation. Strong irritant.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, B, 781 (bibl, rev)
Shafer, E.C. et al, Z. Kristallogr., 1956, 108, 263 (synth)
D'Yvoire, F., Compt. Rend. Hebd. Seances Acad. Sci. Sect. C, 1972, 275, 949 (ir)
Ronis, M. et al, Bull. Soc. Chim. Fr., 1974, 78 (struct, hydrate)
Gevork'yan, S.V. et al, Geol. Zh., 1974, 34, 27 (polymorphism)
Beilina, A.Z. et al, Zh. Neorg. Khim., 1979, 24, 2255 (synth)
Cheetham, A.K. et al, Nature (London), 1986, 320, 46 (nd, cryst struct)
Gouffon, A. et al, Rev. Chim. Miner., 1986, 23, 99 (mössbauer)
Berthet, P. et al, Mater. Res. Bull., 1988, 23, 1501 (xanes)

AsFeS

IC-000481

Iron arsenide sulfide (FeAsS)

Arsenopyrite. Mispickel

[12068-58-5]

FeAsS

M 162.8

Composition (ratio As:S) variable but ~1. Monoclinic; struct. derived from marcasite but of lower symmetry. Mineral, occurs widely. Principal arsenic ore - arsenic extracted by roasting. Silver-white to grey, opaque, metallic cryst.

[1303-18-0]

Hunt, G.R., Geophysics, 1977, 42, 501 (ir)
Lutz, H.D. et al, Phys. Chem. Miner., 1983, 9, 109 (ir)

AsGa

IC-000482

Gallium arsenide (GaAs)

[1303-00-0]

GaAs

M 144.6

Has zinc blende struct. Synth. from elements in sealed tube or by dec. of organometallic precursors. Widely used semiconductor. Forms mixed cryst. with GaP. Black solid. Mp 1240° n_D 3.30, ΔH_f −83.7 (−74.1) kJ mol^{-1}, S° 63 J K^{-1} mol^{-1}. Band gap 1.39eV. ε 11.3. Thermal expansion 6.86 × 10^{-6} K^{-1}. Sp. Heat 0.325 J g^{-1} K^{-1}. Electron mobility 0.85, hole mobility 0.05 m^2 V^{-1} s^{-1}.

▷ LW8800000.

Goldschmidt, G. et al, Acta Crystallogr., 1958, 11, 369 (cryst struct)
Hilsum, C. et al, Semiconducting III-V Compounds, Pergamon, Oxford, 1961

Willardson, R.K. et al, Compound Semiconductors, Reinhold, 1962 (synth)
Harrison, B.C. et al, Inorg. Chem., 1962, 1, 951 (synth)
Piespergen, U., Z. Naturforsch., A, 1963, 18, 141 (sp heat)
Straumanis, M.E., Acta Crystallogr., 1965, 19, 256 (cryst struct)
Thurmond, C.D., J. Phys. Chem. Solids, 1965, 26, 785 (system with GaP)
Pierron, E.D., Acta Crystallogr., 1966, 21, 290 (thermal expansion)
Tietjen, J.J. et al, J. Electrochem. Soc., 1966, 113, 724 (system with GaP)
Willardson, R.K. et al, Semiconductors and Semimetals, Academic Press, 1966, 1, 2; 1967, 3; 1968, 4; 1984, 20; 1990, 29.
Mooradian, A. et al, Solid State Commun., 1966, 4, 431 (raman)
Van Vechten, J.A. et al, Phys. Rev., 1969, 182, 891 (cryst struct)
Clough, R.B. et al, Trans. Am. Inst. Min., Metall. Pet. Eng., 1969, 245, 583 (ternary systems)
Paulus, K. et al, GaAs Rel. Compds. Inst. Phys. GaAs Rel. Compds. Inst. Phys. Conf. Ser., 1976, 33; 1982, 65; 1984, 74; 1985, 79; 1986, 83; 1988, 96.
Shaulov, Yu.Kh. et al, Russ. J. Phys. Chem. (Engl. Transl.), 1977, 51, 634 (synth)
O'Keefe, M. et al, Acta Crystallogr., Sect. B, 1978, 34, 3519 (cryst struct)
Nakajima, K. et al, J. Electrochem. Soc., 1978, 125, 123 (quaternary system)
Makram-Ebeid, S. et al, Semi-Insulating III-V Materials, Shiva, 1980, 1982.
Look, D.C. et al, Semi-Insulating III-V Materials, Shiva, 1984.
Brice, J.C. et al, Properties of GaAs, Institution Electrical Engineers, 1986.
Grossmann, G. et al, Semi-Insulating III-V Materials, Adam Hilger, Bristol, 1988.

$AsGaO_4$

IC-000483

Gallium arsenate ($GaAsO_4$)

Gallium arsenic oxide ($GaAsO_4$). Arsenic gallium oxide ($AsGaO_4$)

[13811-89-7]

$GaAsO_4$

M 208.6

Low-quartz struct. but several open framework forms obt. in presence of org. amines. Synth. from acid solns. of Ga(*III*) soln. contg. $[AsO_4]^{3\ominus}$ or from Ga_2O_3 + H_3AsO_4 at 1000°. White solid.

Shafer, E.C. et al, J. Am. Ceram. Soc., 1956, 39, 330 (cryst struct)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, 1, 1110.
Chen, J. et al, J. Chem. Soc., Chem. Commun., 1989, 1217 (cryst struct, open framework form)
Chen, J. et al, J. Solid State Chem., 1989, 80, 149 (synth, open framework forms)

AsGe

IC-000484

Germanium arsenide (GeAs)

[12271-72-6]

GeAs

M 147.5

Synth. at 800° from Ge + As. Semiconductor. Cryst. Dec. > 650°.

Hillel, R. et al, Thermochim. Acta, 1980, 38, 259 (synth)
Mentzen, B.F. et al, C.R. Hebd. Seances Acad. Sci., Ser. 2, 1981, 293, 965 (synth, cryst struct)
Mead, D.G., Infrared Physics, 1982, 22, 209 (ir)

$AsHMgO_4$

IC-000485

Magnesium arsenate (1:1), 9Cl

Magnesium hydrogen arsenate. Magnesium hydrogen orthoarsenate

[7778-40-7]

$MgHAsO_4$

M 164.2

Additional hydrates recorded include the hemihydrate.

Monohydrate: [33972-31-5].
Colourless cryst. Metastable at 20°.

Hydrate (2:5): [30621-33-1].
Colourless cryst. Stable at 60°

Tetrahydrate: [28877-83-0].
Synth. by ambient air dehydration of heptahydrate. Orthorhombic.

Heptahydrate: [13520-58-6].
Synth. from Na_2HAsO_4 + $MgSO_4$ aq. Large prisms. Monoclinic. At 100° → dihydrate, and at 200° → monohydrate.

Mineral-form
Brassite
Identical to the tetrahydrate. Found as a specimen coating at sites in Germany. Orthorhombic white cryst.

Mineral-form [1319-39-7]
Rosslerite
Identical to heptahydrate. Occurs as a secondary mineral at sites in Germany and Czechoslovakia. Monoclinic white cryst.

Gmelin Handbook Inorg. Chem., Syst. No. 27, 1939, B, 417 (rev, bibl)
Brasse, R. et al, Bull. Soc. Chim. Fr., 1970, 2449; 1971, 82; 1972, 1761 (synth, cryst struct)
Ferraris, G. et al, Acta Crystallogr., Sect. B, 1973, 29, 286 (cryst struct)
Whitaker, A., Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem., 1973, 137, 194 (cryst struct)
Protas, J. et al, Acta Crystallogr., Sect. B, 1976, 32, 1460 (synth, cryst struct)

$AsHMnO_4$

IC-000486

Manganese(*II*) arsenate(*V*) ($MnHAsO_4$)

$Mn(HAsO_4)$

M 194.8

Anhydrous compd. not known. $MnHAsO_4.nH_2O$ (n = 1 or 4) observed in the $Mn_3(AsO_4)_2$-H_3AsO_4-H_2O system.

Monohydrate: [13446-33-8]. ***Krautite***
AsH_3MnO_5 M 212.8
Synth. by mixing aq. solns. of Na_2HAsO_4 and $MnCl_2$. Good transparent and stable gels formed from $MnCl_2$ and KH_2AsO_4 in freshly-boiled H_2O. Also mineral. Pale rose-coloured cryst. Sl. sol. H_2O. Struct. built up from $MnO_4(OH_2)$ octahedra and $AsO_3(OH)$ tetrahedra. Intercalates linear alkylamines. Thermal dec. at 200° gives $Mn_2As_2O_7$.

Tetrahydrate: Light pink cryst.

Weiser, H.B. et al, J. Phys. Chem., 1924, 28, 28 (synth, gels)
Bhadraver, M.S. et al, Bull. Chem. Soc. Jpn., 1962, 35, 1053 (synth)
Nabar, M.A. et al, Z. Naturforsch., B, 1978, 33, 1108 (data)
Catti, M. et al, Am. Mineral., 1979, 64, 1248 (cryst struct)
Beneke, K. et al, Am. Mineral., 1981, 66, 432 (props)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, C9, 329 (rev, bibl)
Soptrajanov, B., J. Mol. Struct., 1986, 143, 163 (ir)

IC-000487

$AsHMn_4O_{12}Si_3$

Tiragalloite

[75797-77-2]

$HMn_4As[Si_3O_{10}]O_1$ or $Mn_4AsSi_3O_{12}(OH)$

M 587.9

Unbranched oligosilicate (3 SiO_4 tetrahedra per unit). Mineral, occurs in Italy. Small orange grains.

Giramaccioli, C.M. et al. Acta Crystallogr., Sect. B, 1979, **35**, 2287 (*cryst struct*)

Giramaccioli, C.M. et al. Am. Mineral., 1980, **65**, 947 (*cryst struct*)

IC-000488

$AsHNa_2O_4$

Disodium arsenate, 9CI, 8CI

Disodium hydrogen arsenate. Sodium arsenate (Na_2HAsO_4)

[7778-43-0]

Na_2HAsO_4

M 185.9

Commercially available. ^{74}As labelled compd. used as radioactive agent. Wood preservative, bacteriocide, herbicide. White solid. Sol. H_2O (10.1 g per 100 cm^3 at 5°). Yields Tetrasodium drarsenate, IC-000626 at *ca.* 195°.

▷ Highly toxic. CG0875000.

Dihydrate: Lozenge-shaped, colourless cryst.

Pentahydrate: [20670-84-2]

Formed by melting heptahydrate at 60°. Colourless square plates. Mp 67°. At 66-99° dehydrates further.

Heptahydrate: [10048-95-0].

Formed by cryst. at >8°. Commercially available. Prisms. V. sol. H_2O (5.5 g per 100 cm^3 at 0°); spar. sol. EtOH. Mp 40°. Dehydrates at 105° or at 30° *in vacuo*. Monoclinic. Layer struct. in which the two crystallographically independent Na atoms are each coordinated by six O atoms (of H_2O molecules); the octahedra sharing terminal edges. The AsO_4 tetrahedra (As–O 1.66–1.74 pm) lie between the layers, and are linked by H-bonds between arsenate and water molecules.

▷ CG0900000.

Octahydrate: [74193-27-4]

Irregular granules, sometimes prisms.

Dodecahydrate: Formed by low temp. cryst. in. Prisms. Mp 22.2°. (20°). Monoclinic.

[7631-89-2, 13510-46-8]

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 939; *Suppl. Vol.*, 1967, **4**, 1093 (*rev, bibl*)

Franke, M. *J. Pharmacol. Exp. Ther.*, 1916, **38**, 454 (*pharmacol*)

Müller, F.A. *et al. Anal. Chem.*, 1952, **24**, 1253 (*ir*)

Guenot, H., *Bull. Soc. Chim. Fr.*, 1957, 323 (*synth*)

Müller, F.A. *et al. Spectrochim. Acta*, 1960, **16**, 135 (*ir*)

Zhukov, A.P. *et al. J. Chem. Soc., Chem. Commun.*, 1968, 854 (*ngr*)

Ferraris, G. *et al. Acta Crystallogr. Sect. B*, 1970, **26**, 1574; 1971, **27**, 354 (*cryst struct*)

Jouan, T. *et al. Bull. Soc. Chim. Fr.*, 1972, 66 (*synth*)

Isac, W.J. *et al. Inorg. Chem.*, 1972, **11**, 2149 (*ps*)

Okamura, K. *et al. Bull. Chem. Soc. Jpn.*, 1973, **46**, 2981 (*props*)

Vansant, F.H. *et al. J. Mol. Struct.*, 1973, **15**, 423 (*raman*)

Milia, F. *Ferroelectrics*, 1978, **20**, 229 (*As-79 ngr*)

Milia, F. *Phys. Status Solidi B*, 1978, **86**, K119 (*As-75 ngr, polymorphism*)

Wagner, C.D. *et al. Anal. Chem.*, 1980, **52**, 1445 (*auger*)

Mackowiak, M. *et al. Solid State Commun.*, 1981, **38**, 537 (*As-75 ngr*)

Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 1324.

Tabeta, R. *et al. Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)

Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 299.

IC-000489

$AsHO_4Pb$

Lead arsenate ($PbHAsO_4$)

Lead hydrogen orthoarsenate

[7784-40-9]

$PbHAsO_4$

M 347.1

Occurs in nature as mineral. Formerly used as pesticide, herbicide, soil sterilant. White, transparent monoclinic leaflets or fluffy powder. Insol. cold H_2O, sl. sol. hot H_2O, sol. HNO_3. Loses H_2O at 220°(280°), dec. at 720°.

▷ Toxic. CG0980000.

Mineral-form [14758-11-3]

Schultenite

Occurs as a secondary mineral with anglesite, bayldonite and others, in e.g. Namibia. Colourless, transparent, vitreous cryst.

McDonnell, C.C. *et al, J. Am. Chem. Soc.*, 1916, **18**, 2027 (*bibl*)

Gmelin Handbook Inorg. Chem., Syst. No. 47, 1970, **C3**, 896 (*rev, bibl*)

Kroupa, J. *et al, Ferroelectrics*, 1978, **21**, 387 (*ir*)

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 3, 247; **13**, 420; **21**, 266 (*uses*)

Brezina, A. *et al, Krist. Tech.*, 1980, **15**, 1447 (*synth*)

Mackowiak, M. *et al, Physica B+C (Amsterdam)*, 1981, **106**, 421.

Roberts, W.L. *et al, Encyclopedia of Minerals*, Van Nostrand Reinhold, NY, 1990, 771 (*schultenite*)

IC-000490

$AsHO_4Sn$

Tin(*II*) arsenate ($Sn(HAsO_4)$)

Arsenic acid, tin(2+) salt (1:1), 9CI

[14214-97-2]

$SnHAsO_4$

M 258.6

Anthelmintic. Needles.

Berndt, A.F., *Acta Crystallogr., Sect. B*, 1971, **27**, 1837 (*cryst struct*)

Gegenava, A.G., *CA*, 1973, **79**, 111250g; 1974, **80**, 16979p (*synth*)

IC-000491

$AsHO_5Ti$

Titanium(*IV*) arsenate hydroxide ($Ti(AsO_4)(OH)$), 11Cl

[84662-61-3]

$Ti(AsO_4)OH$

M 203.8

Synth. by heating aq. $TiCl_4$ and H_3AsO_4 in a sealed quartz ampoule at 250°/40 atm. White solid which dec. to $Ti_2O(AsO_4)_2$ at 400-580°.

Chernorukov, N.G. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 1728 (*synth, ir, powder struct*)

IC-000492

$AsHO_8P_2$

Arsenic phosphate, 8Cl

[12254-96-5]

$AsH(PO_4)_2$

M 265.9

Behaves as a monobasic acid. From As_2O_5-P_2O_5-H_2O system. Rhombic cryst. Forms dihydrate on exp. to air.

Winkler, A. *et al, J. Polym. Sci., Part C*, 1969, 4283 (*synth, cryst struct*).

IC-000493

AsH_2NaO_4

Monosodium arsenate, 9CI, 8CI

Monosodium dihydrogen orthoarsenate. Sodium arsenate (NaH_2AsO_4)

[10103-60-3]

NaH_2AsO_4

M 163.9

Mp 118°. Thought to exist in monoclinic and orthorhombic modifications.

Monohydrate: [13466-04-1].

Synth. from As_2O_5 + NaOH aq. at 0°. White cryst. powder. May be dehydrated *in vacuo* at 30°, or in air at sl. higher temp. Infinite chains of Na octahedra are bridged by AsO_4 tetrahedra. The four AsO_4 oxygen atoms are coordinated to four different Na atoms leading to 3-D network of tetrahedra and octahedra. As—O 164.5-174.9 pm. May exist in two forms (i) rhombic bipyramids, and (ii) monoclinic prisms. Dehydrates at 100-130°, and at 200-280°, → Sodium arsenenate, IC-000536.

Dihydrate: [74193-26-3].

Synth. from As_2O_5 in NaOH aq. Cryst. (H_2O).

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 945; *Supplement*, Vol. 4, 1967, 1698; *Supplement*, Vol. 5, 1970, 2019 (*rev, bibl*)

Zhukov, A.P. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 854 (*ngr*)

Okumura, A. *et al, Bull. Chem. Soc. Jpn.*, 1973, **46**, 2981 (*props*)

Vansant, F.H. *et al, J. Mol. Struct.*, 1973, **15**, 425 (*raman*)

Ferraris, G. *et al, Atti Accad. Sci. Torino, Cl. Sci. Fis., Mat. Nat.*, 1974, 507 (*cryst struct*)

Tilgner, J. *et al, J. Phys. Chem. Solids*, 1975, **36**, 27

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 581 (*synth, monohydrate*)

Rendle, D.F. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2684 (*cryst struct*)

Sagadieva, A.K. *et al, Zh. Neorg. Khim.*, 1980, **25**, 1129; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 626 (*synth, ir, struct*)

Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 302.

IC-000494

AsH_2O_4Rb

Rubidium arsenate (RbH_2AsO_4)

Monorubidium arsenate, 9CI. Rubidium dihydrogen arsenate

[13464-57-8]

RbH_2AsO_4

M 226.4

Synth. from Rb_2CO_3 + H_3AsO_4. Monoclinic. Sol. H_2O (39.8 g per 100 cm^3). Dec. without melting at 192-264°. At 250° → $RbAsO_3$. Ferroelectric trans. at −173° becoming paraelectric.

Cook, W.R., *J. Appl. Phys.*, 1967, **38**, 1637 (*cryst struct*)

Shklovskaya, R.M. *et al, Zh. Neorg. Khim.*, 1967, **12**, 2340; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 1234 (*synth, ir, struct*)

Deshpande, V.T. *et al, Indian J. Pure Appl. Phys.*, 1968, **6**, 97 (*cryst struct*)

Zhukov, A.P. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 854 (*ngr*)

Nicholson, J.Y. *et al, J. Chem. Phys.*, 1974, **60**, 715 (*pmr*)

Farrall, C.W. *et al, Phys. Rev. B*, 1974, **10**, 882 (*props*)

Hamann, S.D., *High Temp. High Pressures*, 1977, **9**, 63 (*ir, props*)

Perry, R.A. *et al, Thermochim. Acta*, 1979, **30**, 115 (*props*)

Takagi, Y. *et al, Ferroelectrics*, 1984, **55**, 743 (*raman*)

Zhigarnovskii, B.M. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1984, **20**, 1243; *Inorg. Materials (Engl. Transl.)*, 1984, **20**, 1074 (*cryst struct, props*)

Chisler, E.V. *et al, J. Mol. Struct.*, 1987, **177**, 231 (*raman, struct*)

IC-000495

AsH_2O_5P

Arsenic oxide phosphate, 8CI

Arsenic phosphoric oxide (As_2O_5·P_2O_5·$2H_2O$)

[12429-06-0]

$AsO(H_2PO_4)$

M 187.9

Part of As_2O_5-P_2O_5-H_2O system. Monoclinic prisms, when heated at 160° yields Arsenic phosphate, IC-000550.

Dachet, J.P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 1767; 1971, **272**, 925 (*synth, props, cryst struct*)

Dorémieux-Morin, C. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1970, **271**, 1193 (*pmr*)

IC-000496

$AsH_2O_{60}W_{18}^{7\ominus}$

Tungstoarsenate ($H_2AsW_{18}O_{60}^{7\ominus}$)

[Arsenito(5−)]

dihydrosypentapentacontaoxooctadecatungstate(7−), 10Cl

$[H_2AsW_{18}O_{60}]^{7\ominus}$

M 4346.2 (ion)

Heteropolyanion. Prepared by reaction of As_2O_3 with $[WO_4]^{2\ominus}$.

Hepta-NH_4 salt, hexadecahydrate: [71393-15-2].

Yellow cryst. (H_2O).

Jeannin, Y. *et al, Inorg. Chem.*, 1979, **18**, 3010 (*synth, cryst struct*)

IC-000497

AsH_3

Arsine, 9CI, 8CI

Hydrogen arsenide. Arseniuretted hydrogen. Arsenious hydride. Arsenic trihydride. Arsane

[7784-42-1]

AsH_3

M 77.9

Synth. by treatment of metal arsenides with dil. aq. acid solns; As_4O_6 + $LiAlH_4$, $AsCl_3$ + $NaBH_4$. Basis of Marsh test for As. Thermally unstable colourless gas with repulsive odour. Readily oxidised to As_2O_3. As + H_2 formed at 250-300°. V. little tendency to protonate. d $^{-55}$ 1.64. Mp −113.5° (−116.3°). Bp −62.4°, Bp −54.8°. Detected in atmosphere of Saturn and Jupiter.

▷ Extremely toxic by inhalation; flammable in air. CG6475000.

Mellor Compr. Treat. Inorg. Theor. Chem., Longmans, London, 1929, **9**, 48 (*rev, bibl*)

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1932, 201 (*rev, bibl*)

Saalfeld, F.E.S. *et al, Inorg. Chem.*, 1963, **2**, 46, 50 (*synth, mol*)

Inorg. Synth., 1963, **7**, 34, 41; 1972, **13**, 14 (*synth*)

Ebsworth, E.A.V. *et al, Trans. Faraday Soc.*, 1967, **63**, 1071 (*pmr*)

Helmsteger, P. *et al, Phys. Rev. A*, 1971, **3**, 122 (*microwave*)

Deryagykh, G.G. *et al, Zh. Neorg. Khim.*, 1971, **16**, 3157; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 1689 (*mic*)

Wyatt, R.H. *et al, Inorg. Chem.*, 1974, **13**, 1511 (*mic*)

Fowler, B.A. *et al, N. Engl. J. Med.*, 1974, **291**, 1171 (*tox, rev, bibl*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 569 (*synth*)

Helms, D.A. *et al, J. Mol. Spectrosc.*, 1978, **69**, 471 (*mm-wave*)

Carlotti, M. *et al, J. Mol. Spectrosc.*, 1983, **102**, 310 (*ir*)

Lovejoy, C.M. *et al, J. Mol. Spectrosc.*, 1984, **104**, 282 (*ir*)

Gendzicki, M. *et al, Z. Naturforsch., B*, 1984, **39**, 1319 (*pe*)

Berkowitz, J. *et al. J. Chem. Phys.*, 1958, **29**, 1068 (*ms*)
Sax, N.I. *et al. Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 306

IC-000498

$AsH_3O_3S_3$

Arsenodithioic acid, 9CI

Thioarsenic acid ($H_3AsO_2S_2$), 8CI

[50288-27-2]

$As(O)(SH)_2(OH) \rightleftharpoons As(S)(SH)(OH)_2$

M 174.0
Obt. only as conc. soln. in Me_2CO aq. From Trisodium arsenodithioate, IC-000539 + 5*M* HCl in Me_2CO at −78°. Light golden colour in Me_2CO soln. pK_{a1} 2.4; pK_{a2} 7.1; pK_{a3} 10.9.

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 460 (*bibl*)
Schmidt, M. *et al. Z. Anorg. Allg. Chem.*, 1963, **326**, 182 (*synth*)

IC-000499

AsH_3O_3S

Arsenothioic acid, 9CI

Thioarsenic acid (H_3AsO_2S), 8CI

[38904-80-6]

$As(S)(OH)_2 \rightleftharpoons As(O)(OH)_2SH$

M 158.0
Obt. only in conc. aq. soln. From Trisodium arsenothioate, IC-000541 aq. + 2*M* HCl in Me_2CO/ice or from H_3AsO_4 + H_2S. pK_{a1} 3.3; pK_{a2} 7.2; pK_{a3} 11.

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 459
Schmidt, M. *et al. Z. Anorg. Allg. Chem.*, 1963, **326**, 182 (*synth*)

IC-000500

AsH_3O_4

Arsenic acid

Trihydroxidooxidoarsenic(V), Orthoarsenic acid

[7778-39-4]

$(HO)_3As(O)$

M 141.9
Triprotic acid; pK_{a1} 2.20; pK_{a2} 6.78; pK_{a3} 11.29 (H_2O at 25°). Reacts with $Na_2S_2O_3$ or $H_2S \rightarrow As_2S_3$, SO_2 + As_2O_3.

▷CG0100000

Mellor Comp. Treat. Inorg. Theor. Chem. Longmans, London, 1922, **9**, 135 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 337 (*rev, bibl*)
Weyrauch, H. *Acta Crystallogr., Sect. B*, 1968, **24**, 987 (*cryst, struct*)
Lalieu, J.P. *et al. Rec. Chim. Miner.*, 1970, **7**, 317 (*solub*)
Yvanisin, F.H. *et al. J. Min. Struct.*, 1971, **11**, 425, 439 (*raman, struct*)
Brauer, G. *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 580, 581 (*synth*)
Tsuzuki, T. *Inorg. Nucl. Chem. Lett.*, 1976, **12**, 699 (*bibl*)
Lesuffle, M. *et al. Can. J. Chem.*, 1979, **57**, 907 (*ir*)
Rao, Y.S. *et al. Manganese Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 298, 299, 306

$AsH_4^{\oplus}$ IC-000501

Arsonium(1+), 9CI, 8CI

[53250-40-1]

$[AsH_4]^{\oplus}$

M 78.9 (ion)
Iodide: [12588-80-6].
AsH_4I M 205.8
Synth. from AsH_3 + HI.

Dung, J.R. *et al. J. Chem. Phys.*, 1971, **54**, 1033 (*synth, ir, raman*)

IC-000502

AsH_4NO_3

Ammonium arsenenite, 9CI

Ammonium arsenite, 8CI

[13462-94-7]

$NH_4(AsO_2)$

M 124.9
Probably of a polymeric struct. Lit. records different subcell types and space groups. Synth. from As_2O_3 + NH_3 at 280° and 1300 atm., or from As_2O_3 + NH_4OH at 70-80°. Monoclinic (orthorhombic) prismatic needles. Sol. H_2O. Dec. slowly in air → NH_3 + As_2O_3. Aq. solns. are strongly alkaline.

Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 444
Jander, G. *et al. Z. Naturforsch., B*, 1972, **27**, 483 (*synth, cryst struct*)
Lazic, C. *et al. Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1977, **285**, 401 (*synth, cryst struct*)

AsH_6NO_4 IC-000503

Monoammonium arsenate, 9CI, 8CI

Ammonium dihydrogen orthoarsenate. Ammonium arsenate ($(NH_4)H_2AsO_4$)

[13462-93-6]

$(NH_4)H_2AsO_4$

M 158.9
The $AsO_4^{3\ominus}$ tetrahedra have As—O 168.2 pm, and OAsO 4 × 111.08°, 2 × 108.67° Synth. from As_2O_3 + $(NH_4)_2CO_3$ aq.; or from H_3AsO_4 + NH_3. Piezoelectric. Commercially available. Large colourless prisms. Sol. H_2O (33.7 g per 100 cm^3 at 0°, 48.7 g per 100 cm^3 at 20°, 122.4 g per 100 cm^3 at 90°). Exhibits complex structural behaviour between r.t. and 450°, but final product of thermal dec. is As_2O_3. Diamagnetic.

Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 445 (*rev, bibl*)
Cook, W.R. *J. Appl. Phys.*, 1967, **38**, 1637 (*cryst struct*)
Dickens, A.P. *et al. J. Chem. Soc., Chem. Commun.*, 1968, 854 (*supr*)
Khan, A.A. *et al. Acta Crystallogr., Sect. B*, 1973, **29**, 2721 (*synth, cryst struct*)
Hannan, S.D. *Aust. J. Chem.*, 1978, **31**, 11, 1988, **41**, 1935 (*ir*)
Piloyan, B.A. *et al. Thermochim. Acta*, 1979, **30**, 115 (*props*)
Dalal, N.S. *et al. Can. J. Chem.*, 1988, **66**, 2045.
Hayashi, Y. *et al. J. Phys. Soc. Jpn.*, 1988, **57**, 1321 (*raman*)
Fukami, T. *et al. J. Phys. Soc. Jpn.*, 1989, **58**, 3429 (*cryst struct*)

$AsH_3O_3P_2S_6$ IC-000504

Tris(*O,O*-dihydrogen phosphorodithioato-*S,S'*)arsenic

Phosphorodithioic acid, tris(anhydrosulfide) with arsenotrithious acid ($(HS)_3As$, 10CI

$[(HO)_2P(S)S]_3As$

M 462.2

O,O,O',O',O'',O''-Hexaethyl ester: [85961-53-1]. *Tris(O,O-diethyl phosphorodithioato-S,S')arsenic, 11CI*
$C_{12}H_{30}AsO_6P_3S_6$ M 630.6
Yellow cryst. Mp 52°.
O,O,O',O',O'',O''-Hexaisopropyl ester: [85961-59-7]. *Tris[O,O-bis(1-methylethyl) phosphorodithioato-S,S'] arsenic, 11CI*
$C_{18}H_{42}AsO_6P_3S_6$ M 714.7
Yellow cryst. (EtOH aq.). Mp 100°.
O,O,O',O',O'',O''-Hexaphenyl ester: [85961-65-5]. *Tris(O,O-diphenyl phosphorodithioato-S,S')arsenic, 11CI*
$C_{36}H_{30}AsO_6P_3S_6$ M 918.8
Sticky yellow solid.

[65853-26-1, 85961-56-4]

Glidewell, C. *et al, Inorg. Chim. Acta*, 1977, **25**, 159 (*synth, P-31 nmr, struct*)
Chauhan, H.P.S. *et al, Polyhedron*, 1983, **2**, 359 (*synth, pmr, P-31 nmr*)

$AsH_6O_6P_3Se_6$ IC-000505

Tris(*O,O*-dihydrogen phosphorodiselenoato)arsenic, 8CI

Phosphorodiselenoic acid, tris(anhydroselenide) with arsenotriselenous acid, 10CI

$[(HO)_2P(Se)Se]_3As$

M 743.6
Hexaethyl ester: [25669-26-5]. *Tris(O,O'-diethyl phosphorodiselenoato-Se,Se')arsenic*
$C_{12}H_{30}AsO_6P_3Se_6$ M 911.9
Pale yellow cryst. (EtOH). Mp 103°.

Krishnan, V. *et al, Inorg. Chem.*, 1969, **8**, 2337

$AsH_7Mo_{12}O_{40}$ IC-000506

Molybdoarsenic acid ($H_7AsMo_{12}O_{40}$)

$H_7[AsMo_{12}O_{40}]$

M 1873.2
Reduced heteropolyacid with Keggin struct. Dark blue cryst. + xH_2O.

Rocchiccioli-Deltcheff, C. *et al, Inorg. Chem.*, 1983, **22**, 207 (*synth*)

$AsH_9N_2O_4$ IC-000507

Diammonium arsenate, 9CI, 8CI

Diammonium hydrogen orthoarsenate. Ammonium arsenate ($(NH_4)_2HAsO_4$)

[7784-44-3]

$(NH_4)_2HAsO_4$

M 176.0
Monoclinic. Cations and anions held by H-bonding. Mean As—O 169.5 pm, OAsO 109.4°. From As_2O_3 + $NH_4(l)$. Plate-like colourless cryst. (prisms). Antiferroelectric.

▷CG0850000.

Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 443 (*rev, bibl*)
Khan, A.A. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 1889 (*synth, cryst struct*)
Milia, F. *et al, J. Chem. Phys.*, 1977, **66**, 1703 (*nqr*)
Milia, F. *et al, Phys. Status Solidi A*, 1977, **42**, 315 (*pmr*)

$AsH_{11}N_2O_8S$ IC-000508

Ammonium arsenate sulfate, 11CI

Diammonium trihydrogen arsenate sulfate. Ammonium sulfate arsenic acid

[99489-71-1]

$(NH_4)_2(H_3AsO_4.SO_4)$

M 274.0
Ordered struct, otherwise closely related to corresp. mixed phosphate. Monoclinic. Anions linked by two cations. In the tetrahedral anions, As—O 168.6, S—O 147.3 pm, angles: OAsO 109.4°, OSO 109.5°. Synth. by cocryst. of H_3AsO_4 (from As_2O_3 aq. + H_2O_2) + $(NH_4)_2SO_4$. Diamond-like platelets. Dec. at 150° to $(NH_4)_2SO_4$, As_2O_5 and H_2O.

Boubia, M. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 1562 (*synth, cryst struct*)
Botto, I.L. *Thermochim. Acta*, 1988, **132**, 279 (*ir, raman, props*)

$AsH_{12}N_3O_4$ IC-000509

Triammonium arsenate, 9CI, 8CI

Triammonium orthoarsenate. Ammonium arsenate ($(NH_4)_3AsO_4$)

[24719-13-9]

$(NH_4)_3AsO_4$

M 193.0
Trihydrate: [13477-86-6].
Synth. from H_3AsO_4 + KOH + large excess NH_4OH. Transparent plates. Isostructural with corresp. phosphate. Tetrahedral $AsO_4^{3\ominus}$ ion with As—O 167.1-170.0 pm and OAsO 108.5°-110.2°. Arrays of H-bonded infinite columns. At r.t. and in open atm., gradually loses NH_3 and → Diammonium arsenate, IC-000507. In aq. soln., loses NH_3 → Monoammonium arsenate, IC-000503.

Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 444 (*rev, bibl*)
Brauer, G. *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 581 (*synth*)
Hsu, T.H. *et al. Acta Crystallogr., Sect. B*, 1977, **33**, 3947 (*synth, cryst struct*)

$AsH_{12}N_3S_4$ IC-000510

Triammonium arsenotetrathioate, 9CI

Triammonium thioarsenate, 8CI

[60508-75-0]

$(NH_4)_3AsS_4$

M 257.3
Orthorhombic. AsS_4 tetrahedra with As—S 220-226 pm, S...S between two tetrahedra 367 pm. From As_2S_3 + $(NH_4)_2S$ aq. Colourless prisms. Surfaces yellow in air. When heated → As_2S_3 + S + $(NH_4)_2S$.

Schäfer, H. *et al, Z. Naturforsch., B*, 1963, **18**, 665 (*cryst struct*)
Brauer, G. *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 583 (*synth*)
Graf, H.A. *et al, Z. Anorg. Allg. Chem.*, 1976, **425**, 67 (*cryst struct*)

[AsHf] IC-000511

Hafnium arsenides

At least seven phases heave been described; none in great detail.

Hafnium arsenide *(Hf_3As), 11CI* [73468-08-3]
$AsHf_3$ M 610.3

Struct. intermediate between those of Fe_2P and Ti_2P. Synth. like $HfAs$

Hafnium arsenide (*Hf_2As*), *8Cl*
$AsHf_2$ M 431.9
Struct. resembles Ta_2P. Synth. by heating the elements to 900° for 3 d then arc-melting the product.

Hafnium arsenide (*Hf_3As_2*), *11Cl*
As_2Hf_3 M 685.3
Isostructural with Hf_3P_2. Synth. like $HfAs$.

Hafnium arsenide (*HfAs*), *11Cl* [12380-31-3]
AsHf M 253.4
Struct. resembles TiP. Synth. by heating Hf and As at 1000° for 70 h or at 900° for 3 d and arc-melting the product.

Hafnium arsenide (*$HfAs_2$*), *11Cl* [12380-37-9]
As_2Hf M 328.3
$PbCl_2$ struct. Synth. like HfAs.

Jeitschko, W. *et al*, *Monatsh. Chem.*, 1962, **93**, 1284 (*synth, cryst struct, HfAs, $HfAs_2$, Hf_2As, Hf_3As*)
Rundqvist, S. *et al*, *Acta Chem. Scand.*, 1968, **22**, 2395 (*synth, cryst struct, HfAs, $HfAs_2$*)
Willerstroem, J.O. *et al*, *J. Solid State Chem.*, 1980, **31**, 227 (*synth, cryst struct, Hf_2As*)

AsIS — IC-000512

Arsenic iodide sulfide (AsIS), 8Cl
Arsenenathious iodide, 9Cl. Arsenic sulfoiodide. Iodothioxoarsenic(III). *Iodothioxoarsine*
[20678-95-9]

I–As=S

M 233.8
Chain struct. proposed. Vitreous, amorphous, and cryst. forms known. Vapour may be polymeric. Synth. by reaction of As + S + I_2 in sealed quartz tube at 600°, *in vacuo*, → vitreous form. Photosemiconductor. Acicular orange star-like growths or cherry-red needles. Mp *ca.* 200-240°. Glassy form, softening pt. 40-80°, crystallises at 110°. Piezoferroelectric. Paramagnetic.

Trimer: see *2,4,6-Triiodo-1,3,5,2,4,6-trithiatriarsenane*, *IC-000857*

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 461 (*rev, bibl*)
Dembovskii, S.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1229; *Inorg. Materials* (*Engl. Transl.*), 1968, **4**, 1079 (*synth*)
Chernov, A.P. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 383; 1970, **6**, 262; *Inorg. Materials* (*Engl. Transl.*), 1969, **5**, 320; 1970, **6**, 228 (*synth*)
Popolitov, V.I. *et al*, *Kristallografiya*, 1969, **14**, 375; 1973, **18**, 891; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1969, **14**, 312; 1973, **18**, 564 (*synth, props, struct*)
Dembovskii, S.A., *Phys. Chem. Glasses*, 1969, **10**, 73 (*struct*)
Kravchenko, E.A. *et al*, *Phys. Status Solidi*, 1969, **31**, K19 (*nqr*)
Melnichenko, T.N. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 1065; *Inorg. Materials* (*Engl. Transl.*), 1971, **7**, 945 (*synth, props*)
Semin, G.K., *Phys. Status Solidi A*, 1972, **11**, K61 (*nqr*)
Seregin, P.P. *et al*, *Fiz. Khim. Steekla*, 1977, **3**, 512; *Sov. J. Glass Phys. Chem.* (*Engl. Transl.*), 1977, **3**, 470 (*pe*)
Archakov, Yu.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 1107; *Inorg. Materials* (*Engl. Transl.*), 1978, **14**, 790 (*mössbauer*)

AsISe — IC-000513

Arsenic iodide selenide (AsISe), 8Cl
Arsenenaselenious iodide, 9Cl. Iodoselenoxoarsine. Iodoselenoxoarsine(III)
[20678-96-0]

I–As=Se

M 280.7
Synth. by reaction between As + Se + I_2 at 600°/0.001 mm → vitreous form, softening at 85°. Annealing at 120° → cryst. forms. Mp 230-240°.

α-form
Monoclinic: 4 molecules per unit cell. Dark red solid by transmitted light, and metallic in reflected light.

β-form
Cubic: 16 molecules per unit cell metastable form. Mp 221°.

Dembovskii, S.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1229; *Inorg. Materials* (*Engl. Transl.*), 1968, **4**, 1079 (*synth*)
Chernov, A.P. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 383; 1970, **6**, 262; *Inorg. Materials* (*Engl. Transl.*), 1969, **5**, 320; 1970, **6**, 228 (*synth*)
Dembovskii, S.A. *et al*, *Phys. Chem. Glasses*, 1969, **10**, 73 (*props*)
Semin, G.K., *Phys. Status Solidi A*, 1972, **11**, K61 (*nqr*)
Bryukhova, E.V. *et al*, *Zh. Strukt. Khim.*, 1972, **13**, 528; *J. Struct. Chem. USSR* (*Engl. Transl.*), 1972, **13**, 493 (*nqr*)
Bazakutsa, V.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1976, **12**, 995; *Inorg. Materials* (*Engl. Transl.*), 1976, **12**, 834 (*electrophys and optical props*)
Seregin, P.P. *et al*, *Fiz. Khim. Steckla*, 1977, **3**, 512; *Sov. J. Glass Phys. Chem.* (*Engl. Transl.*), 1977, **3**, 470 (*pe*)
Archakov, Yu.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 1007; *Inorg. Materials* (*Engl. Transl.*), 1978, **14**, 790 (*mössbauer*)
Kniep, R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1981, **20**, 212
Arivuoli, D. *et al*, *J. Crystal Growth*, 1988, **88**, 353 (*synth*)

AsITe — IC-000514

Arsenic tellurium iodide (AsITe)

Te=As–I

M 329.4
Synth. from elements at < 600° in sealed tube. Cryst.

Cyclic trimer: *2,4,6-Triiodo-1,3,5,2,4,6-tritelluratriarsenane*
$As_3I_3Te_3$ M 988.2
Said to be stable in the range 230-350°.

Dembovskii, S.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1228; *Inorg. Materials* (*Engl. Transl.*), 1968, **4**, 1079 (*synth*)
Gadzhiev, S.M. *et al*, *CA*, 1972, **77**, 25451.
Archakov, Yu.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 1007; *Inorg. Materials* (*Engl. Transl.*), 1978, **14**, 790 (*pe*)

AsI$_3$ — IC-000515

Arsenic iodide (AsI_3), 8Cl
Arsenous triiodide. 9Cl. Triiodoarsine. Triiodoarsenic(III)
[7784-45-4]

AsI_3

M 455.6
Possibly dimorphic. Rhombohedral, hcp struct. with interatomic distance: As–I 259.1 pm; angle IAsI 99.7°. Synth. from As + I_2, or from As_2O_3 + HCl + HI. Commercially available. Lustrous red or orange-red leaves or platelets (CS_2 or Et_2O); dec. in air → As_2O_3 + I_2. Sol. H_2O, Et_2O, CS_2, xylene, dioxan; spar. sol. conc. HCl. Mp 146° (142°). Bp 403°. ΔH_f° (g) 29 kJ mol^{-1}, −58.2 kJ mol^{-1}.

▷ Poison. CG1950000.

Inorg. Synth., 1939, **1**, 103 (*synth*)
Morino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1966, **39**, 71 (*esf*)
Vashchenko, V.I. *et al*, *Fiz. Tverd. Tela* (*Leningrad*), 1972, **14**, 3665; *Soviet Physics. Solid State*, 1972, **14**, 3068 (*synth*)
Chernov, A.P. *et al*, *Zh. Neorg. Khim.*, 1973, **18**, 2876; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **18**, 1530 (*synth*)
Clark, R.J.H. *et al*, *J. Mol. Spectrosc.*, 1974, **52**, 58 (*raman*)
Hillel, R. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 2458 (*raman*)

Matsumoto, K. *et al*, *Talanta*, 1975, **22**, 695 (*ms*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 575 (*synth*)
Peel, J.B. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1976, **9**, 175 (*pe*)
Enjalbert, R. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 914 (*cryst struct*)
Galy, J. *et al*, *J. Solid State Chem.*, 1982, **44**, 1 (*cryst struct, rev*)
Grodzicki, M. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1319 (*pe*)
Dunstan, P.O. *et al*, *J. Chem. Eng. Data*, 1988, **33**, 93 (*complexes*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 303.

$AsI_4^\oplus$ — IC-000518

Tetraiodoarsonium
Tetraiodoarsenic(V)(*I* +)

$[AsI_4]^\oplus$ (T_d)

M 582.5 (ion)
Tetrachloroaluminate:
$AlAsCl_4I_4$ M 751.3
Highly unstable, identified at low temps. by Raman spectrosc.
▷ Dec. explosively > −78°.

Tornieporth-Oetting, I. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 1671 (*synth, raman, haz*)

AsIn — IC-000517

Indium arsenide (InAs)
[1303-11-3]

InAs

M 189.7
Has zinc blende or wurtzite struct. Obt. from elements in 3 zone furnace, or by vapour phase transport using $InCl_3$. Important semiconductor for use at low temps. Commercially available. Black solid. Mp 943°. ΔH_f° −54.4 kJ mol^{-1}; S° 75.8 J K^{-1} mol^{-1}. Band gap 0.36 eV. Refractive index *n* 3.42. ε 12.3. Electron mobility 3.3, hole mobility 0.046 m^2 V^{-1}s^{-1}.

Giesecke, G. *et al*, *Acta Crystallogr.*, 1958, **11**, 369 (*cryst struct*)
Hilsum, C. *et al*, *Semiconducting III-V Compounds*, Pergamon, Oxford, 1961.
Willardson, R.K. *et al*, *Compound Semiconductors*, Reinhold, 1962 (*synth*)
Piespergen, U., *Z. Naturforsch., A*, 1963, **18**, 141 (*thermodyn*)
Luzhnaya, N.P. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 642 (*phase diagram, AsInSe system*)
Willardson, R.K. *et al*, *Semiconductors and Semimetals*, Academic Press, 1966, **1, 2**; 1967, **3**; 1968, **4**.
Van Vechten, J.A. *et al*, *Phys. Rev.*, 1969, **182**, 891 (*cryst struct*)
O'Keefe, M. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3519 (*cryst struct*)
Nakajima, K. *et al*, *J. Electrochem. Soc.*, 1978, **125**, 123 (*quaternary system*)

$AsInO_4$ — IC-000518

Indium(*III*) arsenate
[59150-90-2]

$InAsO_4$

M 253.7
Synth. from $InCl_3$ + H_3AsO_4 at pH 1.9-2.7. Amorphous precipitate loses H_2O at 230-300° and crystallises at 520°. White solid.

[21687-70-7]

Deichmann, E.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 19 (*synth, ir*)

[AsIr] — IC-000519

Iridium arsenides

Iridium arsenide (*IrAs*) [62828-56-2]
AsIr M 267.1
Found as a phase in IrAs semiconductors.

Iridium arsenide (*$IrAs_2$*), *8Cl* [34312-54-4]
Iridium diarsenide
As_2Ir M 342.0
Has the $CoSb_2$ type struct.

Iridium arsenide (*$IrAs_3$*) [12256-08-5]
Iridium triarsenide
As_3Ir M 416.9
Has cubic $CoAs_3$ (skutterudite) struct. (See under Cobalt arsenides, IC-000459).

Heyding, R.D. *et al*, *Can. J. Chem.*, 1961, **39**, 955 (*IrAs, synth, struct*)
Bennett, S.L. *et al*, *Can. J. Chem.*, 1966, **44**, 3017 (*$IrAs_2$, synth, struct*)
Kjekshus, A., *Acta Chem. Scand.*, 1971, **25**, 411 (*$IrAs_2$, $IrAs_3$, synth, struct, magnetism*)
Kjekshus, A., *Acta Chem. Scand., Ser. A*, 1974, **28**, 99.

AsKMnS$_3$ — IC-000520

Manganese potassium arsenide sulfide

$KMnAsS_3$

M 265.1
No recent work. Synth. by reaction of $Mn^{2\oplus}$ soln. with conc. K_3AsS_3 soln. Rapidly dec. to $Mn_3(AsS_3)_2$ in H_2O.

Wunschendorff, H. *et al*, *Bull. Soc. Chim. Fr.*, 1933, **53**, 1529 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 369 (*rev, bibl*)

$AsKO_2$ — IC-000521

Potassium arsenenite, 9Cl
Potassium arsenite, 8Cl. Potassium metaarsenite. Arsenic potassium oxide (*$AsKO_2$*)
[13464-35-2]

$KAsO_2$

M 146.0
Polymeric struct. Synth. from As_2O_3 + K_2SO_4 or $K_2S_2O_7$ at 500-900°.

Monomeric-form
By vaporisation of $KAsO_2$ or K_2CO_3-As_2O_3 mixt., with condensation in N_2 matrix. Thought to consist of $K(O)_2As$ four-membered ring.

Ogden, J.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 825 (*synth, ir, struct*)
Bencivenni, L. *et al*, *J. Mol. Struct.*, 1983, **99**, 23 (*synth, ir, struct*)

$AsKO_3$ — IC-000522

Potassium arsenenate, 9Cl
Potassium arsenate (*$AsO_3^{1\ominus}$*), *8Cl. Potassium metaarsenate*
[19197-73-0]

$KAsO_3$

M 162.0
Exists in several modifications. A molecular form has also been isol. in N_2 matrix. By pyrolysis of KH_2AsO_4 at 550-600° → γ form, KO_2 + As_2O_5 → β-form at ca. 200°. Solid. Mp 660° (640°). ΔH_f° −558 kJ mol^{-1}. β-form → α-form at 520°.

Belina, A.Z. *et al*, *Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1976, **50**, 148 (*ir, raman*)

Isobaev, S.M. *et al. Izv. Akad. Nauk SSSR Neorg. Mater.*, 1977, **13**, 867 (*energy, Mössbauer*) (*Engl. Transl.*) 1977, **13**, 414 (*e*)
Dmitrenko, O. *et al. Rev. Chim. Miner.*, 1978, **15**, 369 (*struct, cryst struct*)
Varvell, H., *Appl. Spectrosc.*, 1979, **33**, 509 (*synth, ir, raman*)
Kanatzidis, B.K. *et al. Z. Naturforsch. B*, 1979, **53**, 2173; *Rev. J. Phys. Chem.* (*Engl. Transl.*), 1979, **53**, 1242 (*synth*)
Ogden, J.S. *et al. J. Chem. Soc., Dalton Trans.*, 1983, 851 (*synth, ir*)
Bensmann, L. *et al. Inorg. Chim. Acta*, 1984, **85**, L11 (*synth, ir*)

IC-000523

AsKSe$_3$

Potassium arsenotriselenoate, 9CI

Potassium triselenoarsenate. Potassium arsenic selenide ($KAsSe_3$)

[104302-49-0]

$KAsSe_3$

M 350.9

Struct. isotypic with corresp. Rb and Cs salts. Synth. from As_2Se_3 + $(NH_4)_2CO_3$ aq. at 135°

Monohydrate

AsH_2KOSe_3 M 368.9

Monoclinic. Pseudo-$AsSe_3$ tetrahedra (As—Se 231.9-242.5 pm) are linked through Se—Se bonds (234.8 pm) into infinite $AsSe_3^-$ chains.

Sheldrick, W.S. *et al. Z. Anorg. Allg. Chem.*, 1986, **535**, 179 (*synth, cryst struct*)

IC-000524

|AsMn|

Manganese arsenides

Manganese arsenide* (Mn_3As), *11CI [61219-26-9]

$AsMn_3$ M 239.7

Has chain struct. Synth. by heating Mn and As under a protective flux or in a corundum crucible in a sealed silica tube. Metallic orthorhombic cryst.

Manganese arsenide* (Mn_2As), *11CI, 10CI [12005-96-8]

$AsMn_2$ M 184.7

Exists in two modifications: tetragonal Cu_2Sb type under ordinary conditions and Fe_2P type at high pressures. Struct. contains Mn atoms with tetrahedral and square-pyramidal As coordination. Obt. by heating stoichiometric amounts of Mn and As powders in an evacuated sealed tube. Cryst., rel. stable in air and HCl. Sol. HNO_3. Antiferromagnetic below 570K. Forms solid solns. with arsenides of type M_2As and Mn_2Sb.

Manganese arsenide* (Mn_2As_3), *11CI, 10CI [12313-65-4]

As_2Mn_4 M 314.6

Distorted cubic struct. Obt. by heating a stoichiometric mixture of powdered Mn and As in an evacuated, sealed quartz tube slowly to 900°. Sol. HNO_3; rel. stable in air and HCl. Ferromagnetic.

***Manganese arsenide* (Mn_4As_3)**

As_3Mn_4 M 444.5

Healing a mixture of powdered MnAs and Mn in a sealed ceramic (Mg_2SiO_4) tube at 1000° gives a product of composition v. close to Mn_4As_3.

Manganese arsenide* (*MnAs*), *10CI [12005-95-7]

AsMn M 129.8

Prepared from elements at 700° for 10h. Whiskers, single cryst., and films have also been prepd. Metallic conductor. Can be ferromagnetic in low temp. hexagonal phase and (under high press.) in the orthorhombic phase. Potential use in magnetooptic storage devices. Commercially available. Greyish-black powder. Mp 936° (As press. 30mm Hg). Paramagnetic above *ca.* 320K.

Guilland, C. *et al, Rev. Metall. (Paris)*, 1948, **45**, 271 (*struct, Mn_2As_3*)
Nowotny, H. *et al, Monatsh. Chem.*, 1951, **82**, 513 (*synth, Mn_3As_2, cryst struct*)
Willis, B.T.M. *et al, Proc. Phys. Soc. B (London)*, 1954, **67**, 290 (*cryst struct, MnAs*)
Yuzuri, M. *et al, J. Phys. Soc. Jpn.*, 1960, **15**, 1845 (*synth, Mn_4As_3*)
Rundqvist, S. *et al, Ark. Kemi.*, 1962/63, **20**, 67 (*cryst struct, Mn_2As*)
Brauer, J.B., *CA*, 1963, **58**, 6527 (*struct, Mn_2As_3*)
Wilson, R.H. *et al, Acta Crystallogr.*, 1964, **17**, 95 (*cryst struct, MnAs*)
Juza, R. *et al, Z. Anorg. Allg. Chem.*, 1964, **331**, 187 (*synth, Mn_2As*)
Hollan, L., *Ann. Chim. (Paris)*, 1966, **1**, 437 (*synth, Mn_2As*)
Ishizawa, Y. *et al, J. Phys. Soc. Jpn.*, 1966, **21**, 189 (*magnetism, Mn_2As*)
Jeitschko, W. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 1971 (*synth, cryst struct, Mn_2As*)
Yuzuri, M., *Phys. Abstr.*, 1972, **75**, 51411 (*esr, synth, Mn_4As_3, Mn_2As_3*)
Selte, K. *et al, Acta Chem. Scand., Ser. A*, 1974, **28**, 61 (*synth, MnAs*)
Selte, K. *et al, J. Phys. Chem. Solids*, 1977, **38**, 719 (*cryst struct, MnAs*)
Kanomata, T. *et al, J. Phys. Soc. Jpn.*, 1977, **43**, 1178 (*magnetism, nd, Mn_2As*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 240 (*rev, bibl*)

IC-000525

AsMnNa

Manganese(*II*) sodium arsenide (MnNaAs)

NaMnAs

M 152.8

Isomorph. with NaMnP, KMnP, KMnAs, NaMnSb, KMnSb, NaMnBr and KMnBi. Tetragonal struct. Na—As 302.4, 314.3, Mn—As 258.6 pm. Synth. by heating elements at 800° for 15 hr in Ar atm. Air- and moisture-sensitive shining black or silvery cryst. Sol. conc. HNO_3, mixts. of conc. HNO_3 + H_2SO_4.

Schuster, H.U. *et al, Z. Naturforsch., B*, 1978, **33**, 113 (*synth, props*)
Achenbach, G. *et al, Z. Anorg. Allg. Chem.*, 1981, **475**, 9 (*synth, cryst struct, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 294 (*rev, bibl*)

IC-000526

|AsMnP|

Manganese arsenide phosphide

$MnAs_{1-x}P_x$

The MnAs-MnP system has been investigated by x-rays and magnetically. When $0 < x \leqslant 0.03$ orthorhombic and hexagonal phases exist. When $0.03 < x < 0.47$ orthorhombic MnP and hexagonal NiAs phases exist. Synth. from MnP, Mn and As at 800° *in vacuo*.

Berg, H. *et al, Philos. Mag.*, 1975, **31**, 1049 (*elec cond*)
Haneda, S. *et al, J. Phys. Soc. Jpn.*, 1977, **42**, 31; 1979, **46**, 802 (*synth, struct, magnetism, electronics*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 384 (*rev, bibl*)

IC-000527

AsMnTi

Manganese titanium arsenide, 10CI

[37215-36-4]

TiMnAs

M 177.7

Possesses hexagonal Fe_2P-type structure like Mn_2P and TiMnP. Prepared from elements at 750-850° followed by long annealing at 850°. Cryst. Other MMnAs, M = V, Cr, Mn, Fe, Co, Ni exist. Pressure-temp. magnetic phase diagram for $Ti_xMn_{1-x}As$ solid solns. has been determined.

Roy-Montreuil, J. *et al, Mater. Res. Bull.*, 1972, **7**, 813 (*synth, cryst struct*)
Sénateur, J.P. *et al, J. Phys. (Paris)*, 1977, **38**, *Suppl.* C7-61 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 302 (*rev, bibl*)

IC-000528

AsMnV

Manganese vanadium arsenide, 10CI

[37215-37-5]

VMnAs

M 180.8

Isomorphous with tetragonal Mn_2As. Synth. from elements at 750-850° followed by long annealing at 850°. Solid. Magnetic properties of $V_{1-x}Mn_xAs$ system have been studied.

Roy-Montreuil, J. *et al, Mater. Res. Bull.*, 1972, **7**, 813 (*synth, struct*)
Selte, K. *et al, Acta Chem. Scand., Ser. A*, 1976, **30**, 8 (*magnetism*)
Sénateur, J.P. *et al, J. Phys. (Paris)*, 1977, **38**, *Suppl.* C7-61 (*props*)
Selte, K., *J. Phys. Chem. Solids*, 1977, **38**, 719 (*magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 305 (*rev, bibl*)

IC-000529

$AsMn_2Sb$

Manganese antimony arsenic

As_xMnSb_{1-x}

M 306.5

MnSb and MnAs form a continuous series of solid solns. with NiAs struct. type. For compositions near MnAs the lattice changes to orthorhombic MnP symmetry. Synth. from pressed powdered elements at 800° for 2 days. Cryst. Exhibits paramagnetic and ferromagnetic behaviour depending on temp. and composition.

Edwards, L.R. *et al, Phys. Rev. B*, 1972, **5**, 1064 (*magnetism*)
Haneda, S. *et al, J. Phys. Soc. Jpn.*, 1979, **46**, 802 (*synth, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 449 (*rev, bibl*)

IC-000530

$AsMn_3N$

Manganese arsenide nitride, 8CI

[12523-18-1]

Mn_3AsN

M 253.7

Tetragonal perovskite type struct. Synth. by heating manganese nitride, Mn, and As in sealed silica ampoules *in vacuo* at 500-800°. Mn_3AsN and Mn_3SbN form a continuous series of solid solns.

Barberon, M. *et al, Mater. Res. Bull.*, 1970, **5**, 1; 1972, **7**, 109 (*cryst struct, synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 365 (*rev, bibl*)

IC-000531

|$AsMn_4Sb$|

Manganese arsenide antimonide

$Mn_2As_xSb_{1-x}$

Mn_2Sb and Mn_2As form a continuous series of solid solns. as shown by neutron and X-ray diffraction measurement. Synth. by heating appropriate portions of elements at 700° for 50h *in vacuo*. Solid solns. crystallise in the tetragonal Cu_2Sb struct. type.

Shirakawa, K. *et al, J. Phys. Soc. Jpn.*, 1976, **40**, 666 (*synth, struct, magnetism*)
Ryzhkovskii, V.M. *et al, Phys. Status Solidi A*, 1978, **47**, K177 (*elec resistivity*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 441 (*rev, bibl*)

IC-000532

$AsMo_{12}O_{40}^{4\ominus}$

Molybdoarsenate ($AsMo_{12}O_{40}^{4\ominus}$), 9CI

[μ_{12}-Orthoarsenato(3 –)]tetracosa-μ-oxododecaoxododecamolybdate(4 –), 11CI

[76130-01-3]

$[AsMo_{12}O_{40}]^{4\ominus}$

M 1866.1 (ion)

Reduced heteropolyanion (heteropolyblue) with α-Keggin struct. (see Tungstosilicate ($SiW_{12}O_{40}^{4\ominus}$), IC-021712 for description). Blue. Obt. electrochemically in soln. and not generally isol.

Jeannin, Y. *et al, Nouv. J. Chim.*, 1980, **4**, 587 (*electronic struct*)
Sanchez, C. *et al, J. Am. Chem. Soc.*, 1982, **104**, 3194 (*synth, esr, uv-vis, bonding*)

IC-000533

$AsMo_{12}O_{40}^{3\ominus}$

Molybdoarsenate ($AsMo_{12}O_{40}^{3\ominus}$), 9CI

[μ_{12}-Orthoarsenato(3 –)]tetracosa-μ-oxododecaoxododecamolybdate(3 –), 11CI

$[AsMo_{12}O_{40}]^{3\ominus}$

M 1866.1 (ion)

Heteropolyanion with Keggin struct. (see Tungstosilicate ($SiW_{12}O_{40}^{4\ominus}$), IC-021712 for a description).

α-form

Tri-Li salt: Yellow powder. Polarog. shows 5 reductions as expected (+0.36, +0.245, +0.02, −0.13, −0.23 vs SCE).

Tris-tetrabutylammonium salt: [81158-05-6] Yellow salt ($MeCN/Et_2O$).

β-form

Tris-tetrabutylammonium salt: Orange-yellow solid.

Akimoto, M. *et al, J. Catal.*, 1981, **72**, 83 (*use*)
Sanchez, C. *et al, J. Am. Chem. Soc.*, 1982, **104**, 3194 (*synth, ir, electrochem*)
Rocchiccioli-Deltcheff, C. *et al, Inorg. Chem.*, 1983, **22**, 207 (*ir, raman, electrochem, thermal anal*)

IC-000534

AsN

Arsenic nitride, 9CI, 8CI

[26754-98-3]

AsN

M 88.9

Formed by microwave discharge through $AsCl_3$ + N_2 mixture.

Jones, W.E., *J. Mol. Spectrosc.*, 1970, **34**, 320 (*formn, uv*)
Fémelat, B. *et al, J. Mol. Spectrosc.*, 1974, **49**, 388 (*form*)

Krishnamurty, G. *et al*, *Indian J. Pure Appl. Phys.*, 1976, **14**, 236 (*formn, str*)
Pillai, P.P., *Indian J. Pure Appl. Phys.*, 1978, **16**, 704.

IC-000535

$AsNaO_2$

Sodium arsenenite, 9CI

Sodium arsenite, 8CI. Sodium metaarsenite. Arsenic sodium oxide ($AsNaO_2$). Arsenious acid ($HAsO_2$) sodium salt, 8CI

[7784-46-5]

$NaAsO_2$

M 129.9

Orthorhombic. Each As is at the apex of a triangular pyramid having 3 oxygens as the base. Each AsO_3 group shares oxygens to form polymeric chains. Synth. from AsO_3—NaOH melt. Commercially available. Herbicide. Used in electroplating of coinage metals. Thin flakes (from melt). V. sol. H_2O; spar. sol. EtOH.

▷ V. toxic. CG3675000.

Tetrahydrate: [111373-27-4].
Synth. from Na_2O—As_2O_3—H_2O system at 6°. The polymetaarsenite anion consists of doublets of single —(O—As)— chains with As—O 183.0-183.8 pm (chain), 171.2 pm (terminal).

Monomeric-form
Synth. by vaporisation of Na_2CO_3—As_2O_3 mixture. May possess a 4-membered $As(O)_2Na$ ring system.

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 935; *Suppl. Vol.*, 1967, **4**, 1687 (*rev, bibl*)
Murray, J.W., *Acta Crystallogr.*, 1958, **11**, 742 (*cryst struct*)
Miller, F.A. *et al*, *Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Wagner, C.D. *et al*, *Anal. Chem.*, 1972, **44**, 967; 1980, **52**, 1445 (*pe, auger*)
Stec, W.J. *et al*, *Inorg. Chem.*, 1972, **11**, 219 (*pe*)
Copenhafer, W.C. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3776 (*O-17 nmr*)
Ogden, J.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 825 (*synth, ir, struct*)
Sheldrick, W. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **549**, 177 (*synth, cryst struct*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3145D.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3045.

$AsNaO_3$

IC-000536

Sodium arsenenate, 9CI

Sodium metaarsenate

[15120-17-9]

$NaAsO_3$

M 145.9

Polymeric substance. Triclinic. Triple chains of tetrahedral AsO_4 groups sharing common corners alternate with $Na^{\oplus}$ layers. Six oxygen atoms form distorted octahedron around each Na. As—O 167-179 pm. By dec. of NaH_2AsO_4 at 270-550°, or $Na_3AsO_4 + As_2O_5$ at melt. Needle-like fibrous hygroscopic cryst. Sol. H_2O. Mp 615° (600°). Exhibits a structural transition at 420° and at >625° → Tetrasodium diarsenate, IC-000626.

▷ Poison. CG1200000

[73938-92-8; 73938-93-9; 73938-94-0]

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 948; *Suppl. Vol.*, 1967, **4**, 1701 (*rev, bibl*)
Nelson, O.A., *J. Am. Chem. Soc.*, 1941, **63**, 1870 (*synth*)
Liebau, F., *Acta Crystallogr.*, 1956, **9**, 811 (*cryst struct*)
Buketov, E.A. *et al*, *Vestn. Akad. Nauk Kaz. SSR*, 1973, **29**, 30; *CA*, **79**, 61104 (*synth*)
Beilina, A.Z. *et al*, *Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 148 (*ir, raman*)
Isabaev, S.M. *et al*, *Zh. Neorg. Khim.*, 1976, **21**, 3134; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1728 (*props, ir, raman*)
Kasenov, B.K. *et al*, *Zh. Fiz. Khim.*, 1979, **53**, 2173; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1979, **53**, 1242 (*props*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 301 (*tox*)

IC-000537

$AsNaS_2$

Sodium arsenenodithioite, 9CI

Sodium thioarsenite, 8CI. Sodium metadithioarsenite. Arsenic sodium sulfide ($AsNaS_2$)

[19102-63-7]

$NaAsS_2$

M 162.0

Monoclinic. Anions are AsS_3 pyramids with common corners forming infinite AsS_2 chains with bridging As—S 231-233 pm, and terminal As—S 217 pm; SAsS angle 95.5°. From $As_2S_3 + Na_2S$ at 100° in sealed tube; or from $As_2S_3 + Na_2CO_3$ at 250-380° in sealed tube; or from $NaAsO_2 + H_2S$. Colourless solid. ΔH°_{298} −283.4 kJ mol^{-1} (from elements). In N_2 at 420°, → Trisodium arsenotrithioite, IC-000543 + As_2S_3. In dry O_2 at 400° → $Na_2SO_4 + As_2O_3 + SO_2$.

Gmelin Handbook Inorg. Chem., Syst. No. 21, *Suppl. Vol.*, 1967, **4**, 1704 (*rev, bibl*)
Palazzi, M. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 3815; 1972, 528 (*synth, cryst struct, props*)
Beilina, A.Z. *et al*, *Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 148 (*ir, raman*)
Palazzi, M. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 908 (*cryst struct*)
Palazzi, M., *Ann. Chim. (Paris)*, 15th Ser., 1978, **3**, 47 (*rev*)
Iglesias, J.E. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1978, **146**, 43 (*cryst struct*)

$AsNa_3OS_3$

IC-000538

Trisodium arsenotrithioate, 9CI

Trisodium trithioarsenate. Sodium trithioarsenate (Na_3AsOS_3)

[26273-99-4]

$Na_3(AsOS_3)$

M 256.0

Orthorhombic. Tetrahedral anion. A hydrate (1:4.5) has been reported. Synth. by dehydration of the undecahydrate. Readily oxidised by H_2O_2 or $K_3Fe(CN)_6$ → As_2S_3 + S.

Nonahydrate: [42282-03-1].
By dehydration of the undecahydrate. Cryst.

Undecahydrate: [42220-65-5].
Synth. from As_2S_3 + NaOH (aq.). Cryst. Orthorhombic.

Thilo, E. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **373**, 111 (*synth*)
Fridman, Ya.D. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 3050; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1589 (*props*)
Palazzi, M., *Bull. Soc. Chim. Fr.*, 1973, 845; 1974, 42 (*synth, cryst struct*)
Palazzi, M., *Ann. Chim. (Paris)*, 15th Ser., 1978, **3**, 37 (*rev*)

IC-000539

$AsNa_3O_2S_2$

Trisodium arsenodithioate, 9CI

Trisodium dithioarsenate. Sodium dithioarsenate ($Na_3AsO_2S_2$)

[38007-31-7]

$Na_3(AsO_2S_2)$

M 240.0

From As_2S_3 + S in NaOH aq. at r.t., or from Na_3AsS_4 in aq. NaOH. Colourless rhombohedral cryst. V. sol. H_2O. In N_2, stable at 330° for 16 hr., but at >500° → $Na_3AsO_4 + Na_3AsS_3$. Reaction with $K_3Fe(CN)_6$ or I_2 → As_2S_5 + S.

Dihydrate: [37807-69-5].
From undecahydrate at r.t. Monoclinic.

Heptahydrate: [37807-68-4].
From undecahydrate at r.t. Monoclinic.

Undecahydrate: [22723-77-9].
Synthesis: As_2S_5 + NaOH aq. at 25°, or Na_3AsS_4 — NaOH aq. Sol. H_2O (35.5 g per 100 cm^3 at 25°). Orthorhombic. Water molecules in two different environments. In the distorted tetrahedral anion, interatomic distances: As—O 169, As—S 212-215, S—O 312-315 pm; angles: OAsO 107.0°, OAsS 109.6°(2×), SAsS 110.8°.

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 955; *Suppl. Vol.*, 1967, **4**, 1706 (*rev, bibl*)
Remy, F., *Bull. Soc. Chim. Fr.*, 1968, 4323 (*cryst struct*)
Fridman, Ya.D. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 3050; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1589 (*props*)
Palazzi, M. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 1772 (*synth, cryst struct*)
Palazzi, M. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 851 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 584 (*synth undecahydrate*)
Jaulmes, S. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 2119 (*cryst struct*)
Palazzi, M., *Ann. Chim. (Paris)*, 15th Ser., 1978, **3**, 37 (*rev, bibl*)

$AsNa_3O_3$

IC-000540

Trisodium arsenite, 9CI

Sodium arsenite (Na_3AsO_3). Sodium orthoarsenite

[13464-37-4]

Na_3AsO_3

M 191.8

Exhibits protective action against Po intoxication in rats. Inhibits oxidative decarboxylation of pyruvic acid.

▷ Highly toxic to mammals and plants.

Hexahydrate: Synth. from As_2O_3 + NaOH aq. + MeOH. Colourless, prismatic needles.

Pietsch, R. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **331**, 344 (*synth*)
Pietsch, R., *Monatsh. Chem.*, 1965, **96**, 138 (*reactions*)
Bhatnagar, C.S. *et al*, *Z. Naturforsch., B*, 1966, **21**, 190 (*formn*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1686 (*rev, bibl*)

$AsNa_3O_3S$

IC-000541

Trisodium arsenothioate, 9CI

Trisodium monothioarsenate. Sodium thioarsenate ($NaAsO_3S$)

[17367-56-5]

$Na_3(AsO_3S)$

M 223.9

Prep. as dodecahydrate which is then dehydrated stepwise under v. mild conditions. A hemihydrate and hexahydrate have also been claimed. Synth. from As_2O_3 + NaOH aq. + S. Colourless hexagonal cryst. Effloresces in air. V. sol. H_2O. In N_2 atm., stable to 420°. At 550°, → $Na_3AsS_3 + Na_2AsO_4$. H_2O → $Na_3AsO_4 + H_2O$. $K_3Fe(CN)_6$ or I_2 → As_2S_5 + S.

Heptahydrate: [34377-63-4].
From dodecahydrate. Monoclinic. Water molecules are sited (in groups of 2 and 5) into two different environments. In AsO_3S irregular tetrahedra, distances: As—O 167, As—S 214, S—O 314 pm; angles: OAsO 107.5-109.3°, OAsS 107.5-113.3°.

Dodecahydrate: [34377-62-3].
Synth. from As_2O_3 + NaOH aq. + S; or from $Na_3AsO_2 + Na_4S_4$; or from As_2S_5 + NaOH aq. Rhomb. bipyramids. V. sol. H_2O (29.5 g per 100 cm^3 at 5°, 80 g per 100 cm^3 at 21°, 100 g per 100 cm^3 at 24°). Orthorhombic. Units of 3 face-sharing distorted $[Na(OH_2)_6]^{\oplus}$ octahedra are each connected by 2 common vertices into zig-zag chains. Endless chains of $[Na_3(OH_2)_{11}]^{3\oplus}$, discrete $AsO_3S^{3\ominus}$ anions, and discrete H_2O molecules, are linked by H-bonds. Better represented as $[Na_3(OH_2)_{11}][AsO_3S]H_2O$. Dehydration under N_2 → heptahydrate.

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 953; *Suppl. Vol.*, 1967, **4**, 1706 (*rev, bibl*)
Fridman, Ya.D. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 3050; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1589 (*props*)
Palazzi, M., *Bull. Soc. Chim. Fr.*, 1971, 1178 (*props, synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 583 (*synth dodecahydrate*)
Palazzi, M., *Acta Crystallogr., Sect. B*, 1976, **32**, 516 (*cryst struct*)
Palazzi, M., *Ann. Chim. (Paris)*, 15th Ser., 1978, **3**, 37 (*rev, bibl*)
Kempa, P.B. *et al*, *Acta Crystallogr., Sect. C*, 1990, **46**, 729 (*cryst struct*)

$AsNa_3O_4$

IC-000542

Trisodium arsenate, 9CI, 8CI

Trisodium orthoarsenate. Sodium arsenate (Na_3AsO_4)

[13464-38-5]

Na_3AsO_4

M 207.8

Thought to exist in low temp. (α, orthorhombic), middle temp. (β, orthorhombic), and high temp. (γ, cubic) forms: transition temps. 410° and 487°. (1:9), (1:7), and (1:3) hydrates also reported. Synth. from H_3AsO_4 + NaOH; or from Na_3AsO_3 + $NaNO_3$. Mp 1260°. Aq. solns. absorb CO_2.

Decahydrate: [28963-25-9].
Synth. by careful dehydration of dodecahydrate. Mp 85°. Cubic. Metastable at amb. temp.

Dodecahydrate: [13510-46-8].
Synth. by reaction of As_2O_3 + Na_2S aq., followed by oxidation. Prismatic granules or slender hexagonal prisms. Mp 66-67° (incongr.). Hexagonal.

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 936; *Suppl. Vol.*, 1967, **4**, 1690; 1970, **5**, 2016.
Tandon, S.P. *et al*, *Indian J. Pure Appl. Phys.*, 1968, **6**, 386 (*str*)
Remy, F. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 2073 (*synth, cryst struct*)
Palazzi, M. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 2795 (*props, struct*)
Stec, W.J. *et al*, *Inorg. Chem.*, 1972, **11**, 219 (*pe*)
Vansant, F.H. *et al*, *J. Mol. Struct.*, 1973, **15**, 425 (*raman*)
Buketov, E.A. *et al*, *Vestn. Akad. Nauk Kaz. SSR*, 1973, **29**, 30; *CA*, **79**, 61104 (*props*)
Beilina, A.Z. *et al*, *Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 148 (*ir,raman*)
Kasenov, B.K. *et al*, *Zh. Fiz. Khim.*, 1979, **53**, 2173; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1979, **53**, 1242 (*props*)

Sagadieva, A.K. *et al, Zh. Neorg. Khim.*, 1980, **25**, 1129; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 626 (*synth, ir, cryst struct*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 301.

IC-000543

AsNa$_3$S$_3$

Trisodium arsenotrithioite, 9CI
Sodium trithioarsenite. Sodium thioorthoarsenite. Sodium arsenic sulfide (Na_3AsS_3)
[16894-55-6]

Na_3AsS_3

M 240.0
Cubic. Anions are individual AsS_3 pyramids, As—S 225 pm, SAsS 101.9°. Mean Na—S 298 pm. A pentahydrate has been reported. From As_2S_3 + Na_2S in solid state. Mp 520° (440°). Stable at 820° for 1 hr. without dec. At 850° → Na_3AsS_2 + S. ΔH°_{298} −684 kJ mol^{-1} (from elements).

Gmelin Handbook Inorg. Chem., Syst. No. 21, Suppl. Vol., 1967, **4**, 1704 (*rev, bibl*)
Palazzi, M., *Bull. Soc. Chim. Fr.*, 1972, 528 (*synth, props*)
Palazzi, M., *Acta Crystallogr., Sect. B*, 1976, **32**, 3175 (*cryst struct*)
Beilina, A.Z. *et al, Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 148 (*ir, raman*)
Sommer, H. *et al, Z. Anorg. Allg. Chem.*, 1977, **430**, 199 (*cryst struct*)
Palazzi, M., *Ann. Chim. (Paris)*, 15th Ser., 1978, **3**, 47 (*rev*)

IC-000544

AsNa$_3$S$_4$

Trisodium arsenotetrathioate, 9CI
Trisodium thioarsenate, 8CI. Sodium tetrathioarsenate (Na_3AsS_4). Sodium arsenic sulfide (Na_3AsS_4)
[16486-45-6]

Na_3AsS_4

M 272.1
Anhydrous salt obt. by dehydration of octahydrate in N_2, or from As_2S_5 + Na_2S in solid state, or by action of H_2S on Na_3AsO_4 in solid state. Mp 620-630°. With O_2 or dry air, → Na_3AsO_4 or Na_2SO_4. ΔH°_{298} −775 kJ mol^{-1} (from elements). $H^\oplus$ → As_2S_5.
Octahydrate: [13472-42-9].
Synth. from As_2S_5 + Na_2S aq. at r.t.; or from Na_3AsO_4 + H_2S at 60°. Pale golden prisms forming colourless aq. solns. Monoclinic: tetrahedral, anion: $Na^\oplus$ ions are each octahedrally coordinated by H_2O and/or S. Isotypic with one form of Na_3PS_4.

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 958; *Suppl. Vol.*, 1967, **4**, 1705 (*bibl, rev*)
Remy, F. *et al, Bull. Soc. Chim. Fr.*, 1968, 3568 (*synth, cryst struct*)
Palazzi, M. *et al, Bull. Soc. Chim. Fr.*, 1969, 3815; 1970, 22 (*synth, cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 583 (*synth*)
Beilina, A.Z. *et al, Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 148 (*ir, raman*)
Palazzi, M., *Ann. Chim. (Paris)*, 15th Ser., 1978, **3**, 37 (*rev*)
Dittmar, J. *et al, Z. Naturforsch., B*, 1978, **33**, 678 (*cryst struct*)
Mereiter, K. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 401 (*raman, cryst struct*)

[AsNb]

Niobium arsenides **IC-000545**

***Niobium arsenide* (Nb_3As)** [12005-98-0]
$AsNb_3$ M 353.6
Isostruct. with Ti_3P. Mixed $(Nb,Ta)_3As$ phases are also known. Synth. by melting Nb and As under 40 atm. Ar or by arc-melting NbAs and Nb.

***Niobium arsenide* (Nb_4As_4)** [12429-24-2]
As_4Nb_7 M 950.0
Struct. like Nb_7P_4. Synth. by arc-melting NbAs and Nb.

***Niobium arsenide* (Nb_5As_3)** [12429-23-1]
As_3Nb_5 M 689.2
Struct. like Nb_5P_3. Synth. by arc-melting NbAs and Nb.

***Niobium arsenide* (Nb_6As_3)** [12429-22-0]
As_3Nb_4 M 596.3
The struct. consists of interconnected Nb_6As trigonal prisms with one extra Nb and one As in holes between the prisms. The coordination number of Nb varies between 4 and 6. Synth. by arc-melting Nb and As.

***Niobium arsenide* (*NbAs*)** [12255-08-2]
AsNb M 167.8
The NbAs struct. type contains $NbAs_6$ octahedra and $AsNb_6$ trigonal prisms; it is related to that of WC. Synth. by thermal dec. of $NbAs_2$ at 1100° or by direct combination of the elements. During formation from the elements a mixture of NbAs and WC structs. is observed.

Boller, H. *et al, Acta Crystallogr.*, 1963, **16**, 1095 (*synth, cryst struct, NbAs*)
Furuseth, S. *et al, Acta Crystallogr.*, 1964, **17**, 1077 (*synth, cryst struct, NbAs*)
Runqvist, S. *et al, Acta Chem. Scand.*, 1969, **23**, 2188 (*synth, cryst structs, various phases*)
Carlsson, B. *et al, Acta Chem. Scand.*, 1971, **25**, 1742 (*cryst struct, Nb_4As_3*)
Waterstrat, R.M. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2765 (*synth, cryst struct, Nb_3As*)
Leohavanich, S. *et al, Acta Crystallogr., Sect. B*, 1981, **37**, 227 (*cryst struct, Nb_5As_3*)
Willerstroem, J.D., *J. Less-Common Met.*, 1984, **99**, 273 (*disorder, NbAs*)

AsNbSi **IC-000546**

Niobium arsenide silicide (NbAsSi), 9CI
Niobium silicide arsenide (111)

NbAsSi

M 195.9
Tetragonal PbFCl struct. Synth. by heating NbSi and As at temps. up to 800°.

Johnson, V. *et al, J. Solid State Chem.*, 1973, **6**, 306 (*synth, cryst struct*)

AsNi **IC-000547**

Nickel arsenide (NiAs), 9CI
Kupfernickel
[27016-75-7]

NiAs

M 133.6
Prototypical layer struct. Other arsenides known, but less studied. Synth. from Ni + As. Red solid. Mp 968°.

Mineral-form
***Niccolite.** Nickeline. Red nickel ore*
Occurs widely. Pale copper-red, metallic solid.

Dana's System of Mineralogy, 7th Ed., Wiley, N.Y, 1944, **1**, 236 (*mineral*)
Remy, H., *Treatise on Inorg. Chem.*, Elsevier, 1956, **2**, 313.

[AsNp] **IC-000548**

Neptunium arsenides

***Neptunium arsenide* (*NpAs*)** [39350-08-8]
AsNp M 311.9
Possesses NaCl struct. Cryst. Semimetallic. Simple ferromagnet at high fields in range 4.2-300K. T_N 173K. Tetragonal struct. at low temps., various phase changes known.

***Neptunium arsenide* ($NpAs_2$)** [39350-10-2]
As_2Np M 386.8
Tetragonal; isostructural with Fe_2As. Cryst. Forms NpAs *in vacuo* at 640°. Ferromagnetic up to 18K, antiferromagnetic 18K-52K, then paramagnetic; μ_{eff} = 1.58μ_B.

Charvillat, J.P. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 337 (*synth*)
Blaise, A. *et al, Solid State Commun.*, 1981, **73**, 659 (*props, magnetism*)
Wojakowski, A. *et al, J. Less-Common Met.*, 1982, **83**, 263 (*synth*)
Delapalme, A. *et al, J. Magn. Magn. Mater.*, 1982, **30**, 117 (*nd*)
Rossat-Mignod, J. *et al, J. Magn. Magn. Mater.*, 1982, **30**, 122 (*nd*)
Boge, M. *et al, J. Magn. Magn. Mater.*, 1982, **30**, 127 (*mössbauer*)
Burlet, P. *et al, J. Less-Common Met.*, 1986, **121**, 325 (*nd*)

AsO$_3$Sb **IC-000549**

Antimony arsenite, 8CI
Arsenic(III) *antimony*(III) *oxide ($AsSbO_3$)*
[12523-20-5]

$AsSbO_3$

M 244.6
Mean interatomic distances: As—O 180, Sb—O 195 pm. Monoclinic. Isostructural with Claudetite I. No As—Sb disorder. Synth. from As_2O_3 + Sb_2O_3 in quartz tube at 400°. Colourless cryst.

Bodenstein, D. *et al, Z. Naturforsch., B*, 1983, **38**, 901 (*synth, cryst struct*)

AsO$_4$P **IC-000550**

Arsenic phosphate, 8CI
Arsenic(III) *phosphoric*(V) *oxide ($As_2O_3 \cdot P_2O_5$)*
[27671-86-9]

$AsPO_4$

M 169.8
Exists in orthorhombic, and other forms. In orthorhombic form, As(*III*) is coordinated by 3 oxygen atoms, the P by 4 oxygen atoms as distorted tetrahedron with interatomic distances: P—O 147.6 - 157.0, As—O 179.4 - 180.0 pm; angles: POP 105.1 - 116.1°, OAsO 89.9 - 90.2°. Synth. from Arsenic oxide phosphate, IC-000495 by heating or from cubic As_2O_3 and hexagonal P_4O_{10}. Weakly hygroscopic cryst.
[13779-14-1]

Dachet, J.P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 1767; 1971, **272**, 925 (*formn, cryst struct*)
Bodenstein, D. *et al, Z. Naturforsch., B*, 1982, **37**, 136 (*synth, cryst struct*)

AsO$_4$Sb **IC-000551**

Antimony arsenate, 8CI
Antimony(III) *arsenic*(V) *oxide*
[28980-47-4]

$SbAsO_4$

M 260.6
Monoclinic. Infinite layer struct. with As tetrahedrally coordinated by four oxygens and Sb coordinated by four oxygens in a one-sided manner. All oxygens bridge As to Sb. Interatomic distances: As—O 163.7, 167.7, 168.6, Sb—O 201.6, 217.4 pm. Synth. by heating Sb_2O_3 + As_2O_5. 5/3 H_2O at 400° for 1week. Alternatively, Sb_4O_6 or As_4O_6 may be used. Air-stable. Colourless rectangular plates.

Jones, P.G. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 1923 (*synth, cryst struct*)

AsO$_9$PZr$_2$ **IC-000552**

[Orthoarsenato(3−)-*O*]-μ-oxo[phosphato(3−)-*O*] dizirconium(*IV*), 11CI
Zirconium arsenate oxide phosphate ($Zr_2(AsO_4)O(PO_4)$)

$(AsO_4)ZrOZr(PO_4)$

M 432.3
Trihydrate: [81899-53-8].
Synth. by mixing aq. solns. of $ZrOCl_2$, Na_2HAsO_4 and Na_3PO_4 at pH 0-1. Acts as an ion-exchanger.

Varshney, K.G. *et al, Sep. Sci. Technol.*, 1981, **16**, 793 (*synth, props*)
Varshney, K.G. *et al, Talanta*, 1983, **30**, 955 (*props*)

AsO$_{11}$PTi$_3$ **IC-000553**

[μ-[Orthoarsenato(3−)-*O*:*O*']]trioxo[μ-[phosphato(3−)-*O*:*O*']]trititanium(*IV*), 11CI
Titanium arsenate oxide phosphate ($Ti_3(AsO_4)O_3(PO_4)$)

$Ti_3(AsO_4)O_3(PO_4)$

M 425.5
Trihydrate: [81899-56-1].
Synth. by mixing aq. solns. of $TiCl_4$ in 30% HCl, with sodium arsenate and sodium phosphate in appropriate proportions. Useful as an ion-exchanger.

Varshney, K.G. *et al, Sep. Sci. Technol.*, 1981, **16**, 793 (*synth, ion-exchange props*)
Varshney, K.G. *et al, Talanta*, 1983, **30**, 955 (*use*)

AsO$_{33}$W$_9^{9\ominus}$ **IC-000554**

Tungstoarsenate ($AsW_9O_{33}^{9\ominus}$), 8CI
μ_9-[Arsenito(3−)]pentadeca-μ-oxopentadecaoxononatungstate(9−), 10CI
[51184-78-2]

$[AsO_{33}W_9]^{9\ominus}$

M 2257.5 (ion)
Heteropolyanion. Formed from As_2O_3 + $[WO_4]^{2\ominus}$ in alk. solns. Forms complex ions with e.g. $Cu^{2\oplus}$.
[77173-96-7, 82975-12-0]

Tourne, C. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1973, **277**, 643 (*synth*)
Robert, F. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 358 (*synth, cryst struct, copper complex*)

AsP **IC-000555**

Arsenic phosphide, 9CI, 8CI
Phosphorus arsenide
[12255-33-3]

AsP

M 105.8

Formed by successive discharge through $AsCl_3$/PCl_3 mixt. or from As_2P fine powder mixt. at 380-550°. Also from AsH_3 + PCl_3 under H_2 and PH_3 + AsF_3 or $AsCl_3$ + PCl_3 at cr. −20°. Brown or red powder. Sol. CS_2, mixt. EtOH, Et_2O, $CHCl_3$. ΔH^o_{298} 187 kJ mol^{-1}. Aerial oxid. → As_2O_3 + P_2O_5.

Gmelin Handbook, Inorg. Chem., Syst. No. 17, 1952, 473 (rev., bibl)
Yoe, K.K. et al, J. Chem. Soc., Dalton Trans., 1969, 586 (form, str)
Ugai, Ya.A. et al, CA, 1971, 74, 36103 (synth)
Gingerich, K.A. et al, J. Phys. Chem., 1974, 78, 603 (ms)
Rassaerts, M. et al, J. Chem. Phys., 1988, 85, 86 (form, str, struct)
Sax, N.I. et al, Dangerous Properties of Industrial Materials, 7th Ed., Van Nostrand-Reinhold, 1989, 304.

IC-000558

AsP_3S_3
3,5,7-Trithia-1,2,4-triphospha-6-arsatricyclo[2.2.1.0^{2,6}]heptane, 11CI
Arsenic phosphorus sulfide (AsP_3S_3)
[85135-63-3]

M 264.0
In equilibrium with Arsenic sulfide (As_4S_3), IC-000666 and Arsenic phosphorus sulfide ($As_2P_2S_3$), IC-000641 or Arsenic phosphorus sulfide ($As_2P_2S_5$), IC-000642 in molten state. Synth. from P_4S_3 + As_4S_3.

Buss, W. et al, Z. Anorg. Allg. Chem., 1984, 516, 42.
Blachnik, R. et al, Z. Naturforsch., B, 1984, 39, 1135 (P-31 nmr)
Baldus, H.P. et al, Monatsh. Chem., 1988, 119, 515 (synth, purif)

AsP_3Se_3 IC-000557

3,5,7-Triselena-1,2,4-triphospha-6-arsatricyclo[2.2.1.0^{2,6}]heptane, 11CI
Arsenic phosphorus selenide (AsP_3Se_3)
[92477-61-7]

M 404.7
Some of reported data may refer to 3,5,7-Triselena-1,2,6-triphospha-4-arsatricyclo[2.2.1.0^{2,6}]heptane, IC-000558. Can be transformed into plastically-cryst. phase by rapid heating of amorphous phase. Synth. from P_4Se_3 + As_4Se_3 as minor isomer. Amorphous or plastic.

Blachnik, R. et al, Z. Naturforsch., B, 1984, 39, 1135 (P-31 nmr)
Blachnik, R. et al, Z. Anorg. Allg. Chem., 1985, 525, 150 (synth, ms, P-31 nmr, hplc)
Baldus, H. et al, Monatsh. Chem., 1988, 119, 515 (synth, hplc)
Tattershall, B.W. et al, J. Chem. Soc., Dalton Trans., 1989, 977 (P-31 nmr, Se-77 nmr)

AsP_3Se_4 IC-000558

3,5,7-Triselena-1,2,6-triphospha-4-arsatricyclo[2.2.1.0^{2,6}]heptane, 11CI
Arsenic phosphorus selenide (AsP_3Se_4)
[92477-62-8]

M 404.7
Some of reported data may refer to 3,5,7-Triselena-1,2,4-triphospha-6-arsatricyclo[2.2.1.0^{2,6}]heptane, IC-000557. Can be transformed into a plastically-cryst. phase by heating amorphous form. Synth. from P_4Se_3 + As_4Se_3 as major isomer. Amorphous or plastic.

Blachnik, R. et al, Z. Naturforsch., B, 1984, 39, 1135 (P-31 nmr)
Blachnik, R. et al, Z. Anorg. Allg. Chem., 1985, 525, 150 (synth, hplc)
Baldus, H. et al, Monatsh. Chem., 1988, 119, 515 (synth, hplc)
Tattershall, B.W. et al, J. Chem. Soc., Dalton Trans., 1989, 977 (P-31 nmr, Se-77 nmr)

[AsPa] IC-000559

Protactinium arsenides

Protactinium arsenide (PaAs) [72931-48-7]
AsPa M 305.9

Protactinium arsenide (Pa_3As_4) [66456-76-6]
As_4Pa_3 M 992.7
Isostructural with Th_3P_4.

Protactinium arsenide ($PaAs_2$) [66341-43-3]
As_2Pa M 380.8
Isostructural with anti-Fe_2As. Exhibits temp.-independent paramagnetism.

Hery, Y. et al, Radiochem. Radioanal. Lett., 1978, 32, 283; 1979, 37, 17 (synth, magnetism)
Calestani, G. et al, J. Less-Common Met., 1979, 68, 207.
Calestani, G. et al, J. Phys. Colloq., 1979, 4, 106.
Brooks, M.S.S. et al, Physica B+C (Amsterdam), 1980, 102, 84.

AsPu IC-000560

Plutonium arsenide (PuAs)
[12006-02-9]

PuAs

M 313.9
Has NaCl struct. Grey metallic solid or black powder. Mp 2420° dec., under Ar. Ferromagnetic (T_c 129K). Tends to lose As on heating ≥ 1000°.

Gorum, A.E., Acta Crystallogr., 1957, 10, 144.
Anselm, F., Compt. Rend. Hebd. Seances Acad. Sci. Sect. C, 1963, 256, 2616.
Kruger, U.L. et al, J. Am. Ceram. Soc., 1966, 49, 661.
Kruger, U.L. et al, J. Phys. Chem. Solids, 1967, 28, 2321.
Lam, D.J. et al, Phys. Rev., 1969, 187, 606.
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, 255 (rev)
Clarillet, J.P. et al, Inorg. Nucl. Chem. Lett., 1973, 9, 559 (synth, struct)
Brauer, G., Handbuch Präp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 1313 (synth)
Blaise, A. et al, Solid State Commun., 1977, 13, 555 (magnetism)
Burlet, P. et al, Phys. Rev. B, 1984, 30, 6660 (nd)
Spirlet, J.C. et al, J. Less-Common Met., 1986, 121, 515 (synth)
Mattenberger, K. et al, J. Magn. Magn. Mater., 1986, 54-57, 539 (magnetism)
Weigel, F. et al, The Chemistry of the Actinide Elements, (Eds. Katz, J.J. et al), Chapman and Hall, London, 1986, 679 (rev)

[AsRe] IC-000561

Rhenium arsenides

Rhenium arsenide (Re_3As_7) [12044-64-3]
As_7Re_3 M 1083.0
This appears to be the only stable phase in the Re—As system. $Ru_3Sn_7(Ir_3Ge_7)$ type struct. with Re—As 258.4, 255.9, Re—Re 277.9 pm. Synth. from Re and As in the presence of I_2. Diamagnetic with metallic type conduction.

Wiechman, F. et al, Z. Anorg. Allg. Chem., 1939, 240, 129 (synth)
Wiglowski, S., Pol. J. Chem. (Rocz. Chem.), 1965, 39, 779.
Furuseth, S. et al, Acta Chem. Scand., 1966, 20, 245 (synth, struct)
Jensen, P. et al, J. Less-Common Met., 1969, 17, 455 (cryst struct)
Rühl, R. et al, J. Solid State Chem., 1984, 53, 55 (synth, struct, phases)

[AsRh] IC-000562

Rhodium arsenides

Various other phases known. Synth. by direct combination of the elements.

Rhodium arsenide (Rh_2As) [37342-44-2]
$AsRh_2$ M 280.7
Has fcc, antifluorite struct. Undergoes reversible $\alpha \rightarrow \beta$ modification at ~ 607° (650-700°).

Rhodium arsenide ($Rh_{12}As_7$) [98111-97-8]
As_7Rh_{12} M 1759.3
Disordered struct. closely related to $Cr_{12}P_7$. Previously described as $Rh_{1.7}As$. Synth. from Rh and As in 12:7 ratio at 800°. Host struct. for rare earth elements.

Rhodium arsenide (RhAs) [91094-33-6]
AsRh M 177.8
Orthorhombic.

Rhodium arsenide ($RhAs_2$) [12337-64-3]
Rhodium diarsenide
As_2Rh M 252.7
Has the $CoSb_2$ type struct.

Rhodium arsenide ($RhAs_3$) [12256-11-0]
Rhodium triarsenide
As_3Rh M 327.6
Isostructural with $CoAs_3$ (Skutterudite).

[86510-29-4, 118917-16-1]

Heyding, R.D. et al, Can. J. Chem., 1961, 39, 955 ($RhAs_3$, RhAs, synth, struct)
Claire, J. et al, Can. J. Chem., 1962, 40, 814 ($RhAs_2$, synth)
Kjekshus, A., Acta Chem. Scand., 1971, 25, 411; 1972, 26, 2554 ($RhAs_2$, Rh_2As, synth, struct)
Kjekshus, A., Acta Chem. Scand., Ser. A, 1974, 28, 99 (cryst struct, $RhAs_3$)
Lutz, H.D. et al, Z. Anorg. Allg. Chem., 1981, 480, 105 (ir, $RhAs_3$)
Pivan, J.Y. et al, J. Less-Common Met., 1985, 107, 249 (cryst struct, $Rh_{12}As_7$)
Lambert-Andron, B. et al, J. Less-Common Met., 1985, 108, 353 (cryst struct, $Rh_{12}As_7$)
Secoue, M. et al, J. Crystal Growth, 1986, 76, 135 (synth, Rh_3As)

[AsRu] IC-000563

Ruthenium arsenides

Ruthenium arsenide (RuAs)
AsRu M 175.9
Isostructural with MnP. Prepd. by heating the elements in a sealed tube at 700°. Rhombic cryst.

Mineral: [53172-82-0]. ***Ruthenarsenite, 9CI***
Pale orange brown to grey. Orthorhombic; contains. Ni partially replacing Ru.

Ruthenium arsenide ($RuAs_2$) [12006-30-3]
Ruthenium diarsenide
As_2Ru M 250.9
A compressed marcasite struct. (or löllingite struct.). Prepd. by heating the elements in a sealed tube at 700°. Orthorhombic.

Mineral: [72271-23-9]. *Anduoite, 10CI* [86510-30-7]

Heyding, R.D. et al, Can. J. Chem., 1961, 39, 955 ($RuAs$, $RuAs_2$, struct)
Hulliger, F., Nature (London), 1963, 198, 1081 (magnetism, semiconductivity, $RuAs_2$)
Holseth, H. et al, Acta Chem. Scand., 1968, 22, 3273, 3284 (struct, $RuAs_2$)
Holseth, H. et al, J. Less-Common Met., 1968, 16, 472 ($RuAs$, diamagnetism)
Harris, D.C., Can. Mineral., 1974, 12, 280 (ruthenarsenite)
Tsui, C.H. et al, CA, 1980, 92, 44791n (anduoite)

AsSe IC-000564

Arsenic selenide (AsSe), 9CI
Selenium arsenide (SeAs)
[12006-05-2]

AsSe

M 153.8
From As + Se at 260°. Trigonal. Mp 300°. Softening pt. ca. 170°.

Dembovskii, S.A., Phys. Chem. Glasses, 1969, 10, 73 (props)
Kravchenko, E.A. et al, Phys. Status Solidi, 1969, 31, K19 (ngr)
Gospodinov, G. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1974, 10, 1125; Inorg. Materials (Engl. Transl.), 1974, 10, 962 (synth)
Viktorovskii, I.V. et al, Fiz. Khim. Steckla, 1976, 2, 284; Sov. J. Glass Phys. Chem. (Engl. Transl.), 1976, 2, 279 (magnetic and electrical props)

AsSn IC-000565

Tin arsenide (SnAs)
[12044-32-5]

SnAs

M 193.6
NaCl type struct. Phase in the Sn—SnAs melt system. Semiconductor, exhibits superconductivity. White, lamellar cryst. Mp 610°.

Vasil'ev, L.N. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1971, 7, 2069 (mössbauer)
Vdovina, T.Z. et al, Zh. Neorg. Khim., 1974, 19, 2257; Russ. J. Inorg. Chem. (Engl. Transl.), 1974, 19, 1234 (cryst struct)
Baidakov, L.A. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1977, 13, 616.
Swanson, H.E., NBS Monogr. (U.S.), 1983, 85.

[AsTa] IC-000566

Tantalum arsenides

Tantalum arsenide (Ta_3As), 10CI [12255-41-3]
$AsTa_3$ M 617.7
This phase was reported by Ganglberger to have the Ti_3P struct. Nb_3As and $(Nb,Ta)_3As$ phases have this struct. but more recent work established a new struct for Ta_3As in which there is a network of four octagonal antiprisms of Ta atoms. Synth. by heating Ta and As in a sealed silica tube at 700°.

Tantalum arsenide (Ta_2As) [12429-12-8]
$AsTa_2$ M 436.8
Struct. like Ta_2P. Synth. by arc-melting TaAs and Ta then heat treating in an induction furnace at 1700°.

Tantalum arsenide (Ta_4As_3), 9CI [12429-25-3]
As_4Ta_9 M 1204.4
Struct. resembles Ti_3Te_4. Synth. by dec. of TaAs at 1500°.

Tantalum arsenide (TaAs), IICI [12255-40-2]
AsTa M 255.8
Isostructural with NbAs but WC struct. is found in unannealed samples. Synth. by heating the elements in a sealed silica tube at 700° and annealing at 1200°.

Tantalum arsenide (TaAs$_2$), 10CI [12256-00-7]
As_2Ta M 330.7
Isostruct. with $NbAs_2$. By-product of the reaction of K and As in a sealed Ta tube at 800°.

Ganglberger, E. *et al, Monatsh. Chem.*, 1986, **97**, 1696 (*synth, cryst struct, Ta_2As*)
Rundqvist, S. *et al, Acta Chem. Scand.*, 1969, **23**, 2188 (*synth, cryst struct, Ta_3As*)
Mueller, J.J. *et al, J. Less-Common Met.*, 1976, **46**, 311 (*synth, struct, Ta_3As, Ta_2As*)
Wang, Y. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 1447 (*cryst struct, Ta_3As*)
Ling, R.G. *et al, C.R. Hebd. Seances Acad. Sci. Ser. 2*, 1981, **292**, 891 (*synth, cryst struct, $TaAs_2$*)
Wolfsgruber, L. *J. Less-Common Met.*, 1984, **99**, 333 (*disordr, TaAs*)

IC-000567

AsTe

Arsenic telluride (AsTe), 9CI
Tellurium arsenide
[12044-35-6]

AsTe

M 202.5
Polymorphic. Synth. from As + Te.

Cryst form
Face-centred cubic struct. Mp 362°. Exhibits phase transitions at 122°, 215°, 245°

Quinn, R.K., *Mater. Res. Bull.*, 1974, **9**, 803 (*synth, cryst struct*)
[Note: ICSD *et al, Trans. Am. Crystallogr. Assoc.*, 1974, **11** (*ref. struct*)]
Bolotnikov, L.S. *et al, Fiz. Khim. Stekla*, 1975, **1**, 456; *Sov. J. Glass Phys. Chem. (Engl. Transl.)*, 1975, **1**, 432 (*magnetism, propr*)

[AsTh] **IC-000568**

Thorium arsenids

Thorium arsenide (ThAs) [12255-42-4]
AsTh M 306.9
Has NaCl struct.

Thorium arsenide (As$_2$Th$_3$) [12006-47-2]
As_2Th_3 M 925.8
Isostructural with Th_3P_4. Semiconductor

Thorium arsenide (As$_3$Th)
As_3Th M 381.8
Exists in two cryst. forms: α-form (orthorhombic) stable below 1100° is isostructural with Fe_3As_2; β-form (tetragonal) stable above 1100° is isostructural with $ZrAs_2$.

Fesser, R., *Acta Crystallogr.*, 1955, **8**, 360; 1956, **9**, 817 (*ThAs*)
Cannell, D.J. *et al, J. Chem. Educ.*, 1959, **36**, 499 (*ThAs*)
Price, C.E. *et al, J. Electrochem. Soc.*, 1965, **112**, 510 (*ThAs*)
Hulliger, F., *Nature (London)*, 1966, **209**, 499
Hulliger, F. *J. Less-Common Met.*, 1968, **16**, 113
Benz, R., *J. Nucl. Mater.*, 1968, **28**, 233
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1157 (*synth, ThAs, Th_3As_2, $ThAs_2$*)
Brown, D. *et al, J. Less-Common Met.*, 1978, **61**, 161 (*ThAs*)
Henkie, Z. *et al, J. Phys. Chem. Solids*, 1978, **39**, 39 (*Th_3As_2*)

[AsTi] **IC-000569**

Titanium arsenides

Titanium arsenide (Ti$_5$As$_3$), 10CI [64417-69-2]
As_3Ti_5 M 418.5
Has the Ti_5P_3 struct. Synth. by arc-melting TiAs + Ti in an Ar atm.

Titanium arsenide (Ti$_2$As), 10CI [67115-99-5]
$AsTi_2$ M 170.6
Has the Fe_2As struct. Synth. by arc-melting TiAs and Ti.

Titanium arsenide (Ti$_3$As$_2$), IICI [12256-12-1]
As_2Ti_3 M 464.2
Has the β-Yb_2Sb_3 struct. Synth. by arc-melting slightly impure TiAs in an Ar atm. or by melting TiAs + Ti in an Ar atm. or by melting TiAs + Ti.

Titanium arsenide (Ti$_4$As$_3$), 10CI [64417-66-9]
As_3Ti_4 M 416.3
Has the *anti*-Th_3P_4 struct. Synth. by arc-melting TiAs in an Ar atm.

Titanium arsenide (TiAs), IICI [12255-43-5]
AsTi M 122.8
Has the TiP struct. TiAs forms solid solns. with many binary arsenides. Synth. by reaction of the elements in a silica tube at 700° for 7 days.

Titanium arsenide (TiAs$_2$), 9CI [12006-35-8]
As_2Ti M 197.7
Ti is 8-coordinated in a bicapped trigonal prismatic arrangement. Synth. by heating Ti and As in a silica tube for 30 days.

Kjekshus, A., *Acta Chem. Scand.*, 1972, **26**, 1633 (*synth, cryst struct, $TiAs_2$*)
Sinha, A.K. *et al, Solid-State Electron.*, 1976, **19**, 489 (*formation of TiAs in Ti containing GaAs Schottky diodes*)
Berger, R., *Acta Chem. Scand., Ser. A*, 1977, **31**, 514 (*synth, struct, TiAs, Ti_3As, Ti_4As_3, Ti_5As_3*)
Senateur, J. *et al, J. Phys. Colloq.*, 1977, **C7**, 61 (*cryst struct, Ti_2As*)
Suzuki, T. *et al, J. Appl. Phys.*, 1984, **55**, 2042 (*solid solns of TiAs in Cr-As*)

[AsU] **IC-000570**

Uranium arsenides

[54887-11-3]

Uranium arsenide (UAs) [12255-45-7]
AsU M 372.9
NaCl struct. Mp 2542° (under Ar). Dissociates at lower temps. under equilibrium conditions. Type I Antiferromagnet. Magnetic behaviour parallels uranium phosphide. T_N 127K. Volatile at Mp.

Uranium Arsenide (UAs$_4$) [12006-49-4]
As_4U_3 M 1013.7
Has Th_3P_4 struct. Air-stable iron-grey microcryst. Metallic conductor. μ_{eff} = 2.81 μ_B (θ 200°). Ferromagnetic, T_c 198K. μ_{eff} (ordered) = 1.71μ_B. V. anisotropic magnetisation.

Uranium arsenide (UAs$_2$) [12006-36-9]
Uranium diarsenide
As_2U M 387.8
Struct. resembles Fe_2As. μ_{eff} = 2.94μ_B (θ 34°). antiferromagneitic, T_N 283K. μ_{eff} (ordered) = 1.61μ_B. Strong magnetic anisotropy.
b Not stable in air. Ignites at 550°

Iandelli, A., *Atti R. Accad. Naz. Lincei, Rend. Cl. Sci. Fis., Mat. Nat.*, 1952, **13**, 144 (*struct*)
Trzebiatowski, W. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1964, **12**, 687 (*magnetism, struct*)
Baskini, Y., *J. Inorg. Nucl. Chem.*, 1967, **29**, 2480 (*synth*)
Leciejewicz, J. *et al, Phys. Status Solidi*, 1968, **30**, 157 (*struct*)
Henkie, Z. *et al, Pol. J. Chem. (Rocz. Chem.)*, 1968, **41**, 363.

Buhrer, C.F., *J. Phys. Chem. Solids*, 1969, **30**, 1273.
Leciejewicz, J. *et al, Phys. Status Solidi B*, 1971, **46**, K67 (*magnetism*)
Lander, G.H. *et al, Phys. Rev. B*, 1972, **6**, 1880.
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **5**, 344 (*rev*)
Sechovsky, V. *et al, Phys. Status Solidi A*, 1974, **26**, K13 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1239 (*synth*)
Rivoiry, F. *et al, Phys. Status Solidi A*, 1976, **33**, K15 (*magnetism*)
Busch, G. *et al, J. Phys. (Paris)*, 1979, **4**, 63 (*magnetism*)
Schoenes, J., *Physica B+C (Amsterdam)*, 1980, **102**, 45 (*electronic struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 55, Suppl., 1981, **C14**, 149 (*rev*)
Henkie, Z. *et al, Phys. Rev. B: Condens. Matter*, 1983, **28**, 4198 (*synth, U_3As_4*)
Schoenes, J. *et al, Solid State Commun.*, 1983, **47**, 23 (*U_3As_4*)
Erdős, P. *et al, The Physics of Actinide Compounds*, Plenum, New York, 1987, 22

[AsV] **IC-000571**

Vanadium arsenides

Vanadium arsenide (V$_3$As), IICI [57284-35-2]
AsV_3 M 176.8
Struct. unknown; unit cell is hexagonal. Synth. by arc melting the component elements.

Vanadium arsenide (V$_2$As$_3$), IICI [12256-13-2]
As_3V_2 M 479.4
The α-form is isostructural with α-W_2Bi_3. The β-form has the Y_2Bi_3 struct. while the γ-form is isostructural with β-Yb_2Sb_3; the last two are closely similar and similar to Rh_2Ge_3. The α-form is synth. by arc-melting V + $VAs_{0.95}$; the β-form by heating V + As to 1000° in an evacuated SiO_2 tube; the γ-form by arc-melting V + As.

Vanadium arsenide (V$_3$As$_2$), IICI [12256-02-9]
As_2V_3 M 302.6
Structure comprises bcc arrangement of V with As in a trigonal prismatic array and is related to that of Ti_3Te_4 in which V is in octahedral voids in the latter struct. Synth. by heating V and As in an evacuated SiO_2 tube.

Vanadium arsenide (V$_4$As$_3$), IICI [39357-32-9]
As_3V_4 M 428.5
The α-form has the Nb_3As_3 struct. while the β-form is isostructural with Cr_4As_3. Defect structs. of this phase have been described. The α-form is synth. at rel. low temps. by vapour phase transport and the β-form is obt. by arc-melting the α-form.

Vanadium arsenide (VAs), IICI [12044-34-7]
AsV M 125.8
There is no evidence for magnetic ordering either in susceptibility data or neutron diffraction to 4K. Isostructural with MnP. Synth. by heating V and As to 850° in a sealed SiO_2 ampoule for 8 days then repeatedly annealing. There is no range of homogeneity around the 1:1 composition. Solid solns. $V_{1-x}Ti_xAs$ ($0 < x < 0.23$) are also known and have the MnP struct. $VP_{1-x}As_x$ phases are also known.

Selte, K. *et al, Acta Chem. Scand.*, 1972, **26**, 4507 (*synth, cryst struct, nd, uv-vis, magnetism, VAs*)
Yvon, K. *et al, Monatsh. Chem.*, 1972, **103**, 1643 (*synth, cryst struct, α-V_4As_3*)
Berger, R., *Acta Chem. Scand., Ser. A*, 1974, **28**, 771; 1975, **29**, 641; 1976, **30**, 363; 1977, **31**, 223, 287 (*synth, cryst struct, V_4As_3, V_3As, α and β-V_2As_3, V_2As_3*)
Andersson, S. *et al, J. Solid State Chem.*, 1976, **19**, 169 (*defect struct, α-V_4As_3*)
Fjellvåg, H. *et al, Acta Chem. Scand., Ser. A*, 1986, **40**, 17 (*VAs/TiAs solid solns*)

[AsZn] **IC-000572**

Zinc arsenides

Zinc arsenide (Zn$_3$As$_2$) [12006-40-5]
As_2Zn_3 M 346.0
Exists in α (face-body centred), α′ (tetragonal) and β (fluorite type) forms with transition temps. α → α′ 161°, α′ → β 672°. Synth. from elements. Commercially available. Grey solid; ferroelectric. Mp 1015°.

Zinc arsenide (ZnAs$_2$) [12044-55-2]
As_2Zn M 215.2
Two distinct Zn and 4 distinct As sites; Zn bonded to 4As, As bonded to 2Zn and to 2As; As atoms arranged in semi-spiral chains. No Zn—Zn bonding. Synth. from elements. Used in Zn diffusion doping of group IIIA pnictides. Grey-black orthorhombic cryst. Mp 771° (under As pressure of 3.3 atm.). Subl. at Mp. Semiconductor; cathodoluminescent. Markedly anisotropic w.r.t. optical and elect. props.

von Stranksellberg, M. *et al, Z. Phys. Chem. Abt. B*, 1934, **48**, 421
Gmelin Handbuch Inorg. Chem., Syst. No. 32, 1956, 997 (*rev, bibl*)
Silvey, G.A. *et al, J. Electrochem. Soc.*, 1961, **108**, 653 (*synth, propr*)
Turner, W.J. *et al, Phys. Rev.*, 1961, **121**, 759 (*phys propr*)
Glazov, V.M. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1969, **185**, 141 (*synth, Zn_3As_2*)
Wei, C.-C. *et al, Ts'ai Liao K'o Hsueh*, 1972, **4**, 1 (*Zn_3As_2, elec propr*)
Fleet, M.E., *Acta Crystallogr., Sect. B*, 1974, **30**, 132 (*synth, cryst struct, $ZnAs_2$*)
Pistorius, C.W.F.T., *High Temp. High Pressures*, 1975, **7**, 681 (*phase diagram, polymorphs, Zn_3As_2*)
Dzumashevskaya, E.P. *et al, Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1975, **49** (*pr, $ZnAs_2$*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1033 (*synth, Zn_3As_2*)
Pietrasko, A. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1976, **24**, 459 (*cryst struct, Zn_3As_2*)
Iwami, M. *et al, J. Phys. Soc. Jpn.*, 1976, **41**, 521 (*magnetism, Zn_3As_2*)
Zyubrist, T.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1977, **13**, 355 (*struct, Zn_3As_2*)
Kudintseva, G.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1978, **241**, 1073 (*photoemission*)
Isotov, A.D. *et al, Kristallografiya*, 1978, **23**, 768 (*cryst struct*)
Marenkin, S.F. *et al, J. Crystal Growth*, 1980, **50**, 761 (*synth, cryst growth*)
Sobolev, V.V. *et al, Fiz. Tekh. Poluprov.*, 1981, **15**, 1429 (*reflectance spect, $ZnAs_2$*)
Lazarev, V.B. *et al, Mater. Res. Bull.*, 1981, **16**, 1113 (*phase diagram*)
Sujak-Cyrus, B. *et al, J. Phys. Chem. Solids*, 1982, **43**, 1045 (*opt props, Zn_3As_2*)
Sobolev, V.V. *et al, Zh. Prikl. Spektrosk.*, 1984, **41**, 1035 (*reflectance spect, $ZnAs_2$*)
Gus'kov, V.N. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1987, **23**, 1418 (*phase diagram*)
Sobczak, E. *et al, J. Phys. Colloq. C*, 1987, **9**, 1005 (*uv-vis, pr, Zn_3As_2*)
Garbuzov, V.E. *et al, Zh. Fiz. Khim.*, 1987, **61**, 525 (*heat capacity*)
Schmidt, N.E., *Zh. Fiz. Khim.*, 1987, **61**, 3105 (*phase trans, Zn_3As_2*)
Prikhod'ko, E.V. *et al, Zh. Fiz. Khim.*, 1988, **62**, 62 (*struct, propr*)
Marenkin, S.F. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1989, **25**, 905, 1039 (*synth, optical and elect props*)

[AsZr] **IC-000573**

Zirconium arsenides

At least five phases have been reported but not extensively studied.

Zirconium arsenide (Zr$_3$As), IICI [12255-49-1]
$AsZr_3$ M 348.5
Isostructural with Ti_3P. Synth. by heating the elements in a sealed silica tube.

Zirconium arsenide (Zr_3As_3), *1ICI* [60240-83-7]
As_3Zr_3 M 423.5
Isostructural with Hf_3P_3. Synth. by heating the elements to 900° in a sealed tube and arc-melting the product.

Zirconium arsenide (Zr_5As_3), *1ICI* [60240-84-8]
As_3Zr_5 M 1104.4
Isostructural with Nb_5P_3. Synth. by heating the elements to 900° in a sealed tube and arc-melting the product.

Zirconium arsenide (*ZrAs*), *1ICI* [60909-47-9]
AsZr M 166.1
High temp., α-ZrAs has the NaCl struct., the low-temp. β-form has the TiP struct. Synth. by heating Zr and As in a sealed tube at 900° and arc-melting the product.

Zirconium arsenide ($ZrAs_2$), *1ICI*
As_2Zr M 241.0
$PbCl_2$ struct. Synth. by heating the elements in a sealed tube.

Trzebiatowski, W. *et al*, *Pol. J. Chem. (Rocz. Chem.)*, 1958, **32**, 189; *CA*, **52**, 17879e (*synth, cryst struct, $ZrAs_2$*)
Lundstrom, T., *Acta Chem. Scand.*, 1966, **20**, 1712 (*synth, cryst struct, ZrAs*)
Carlsson, B. *et al*, *Acta Chem. Scand., Ser. A*, 1976, **30**, 386 (*synth, cryst struct, Zr_3As_2, Zr_4As_3*)
Wilhelmsen, J.O., *Acta Chem. Scand., Ser. A*, 1984, **38**, 91 (*synth, cryst struct, ZrAs, Zr_3As_2, Zr_5As_3*)

IC-000574

$As_2B_8H_8S$
8-Thia-7,9-diarsaundecaborane(8), 10CI, 9CI
7,9-Diarsena-8-thiaundecaborane(8)
[51846-24-3]

X = S

M 276.4
nido- Air-sensitive colourless cryst. Sol. MeCN, MeOH, hexane. Mp 386-390° dec. Sublimes.

Siedle, A.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 914 (*synth, ms*)
Barriola, A.M. *et al*, *Inorg. Chem.*, 1980, **19**, 2801 (*synth, B-11 nmr*)

IC-000575

$As_2B_8H_8Se$
8-Selena-7,9-diarsaundecaborane(8), 10CI
7,9-Diarsena-8-selenaundecaborane(8)
[74096-64-3]

As 8-Thia-7,9-diarsaundecaborane(8), IC-000574 with

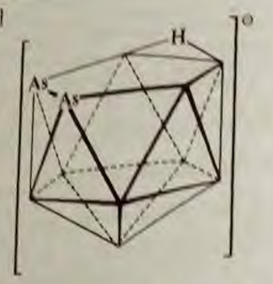
X = Se

M 323.3
nido- Yellow solid. Sol. MeCN, heptane. Mp 427-430°.

Barriola, A.M. *et al*, *Inorg. Chem.*, 1980, **19**, 2801 (*synth, ms, B-11 nmr*)

IC-000576

$As_2B_9H_{10}^{\ominus}$
Decahydro-7,8-diarsaundecaborate(1−), 9CI
[51668-00-9]



M 257.2 (ion)
Me_4N salt: From 1,2-Diarsadodecaborane(10), IC-000577 + piperidine followed by addn. of $[Me_4N]Cl$. Cryst. (Me_2CO/MeOH). Sol. Me_2CO.

Little, J.L. *et al*, *Inorg. Chem.*, 1974, **13**, 1752 (*synth, ir, pmr, B-11 nmr*)
Todd, L.J. *et al*, *Inorg. Chem.*, 1987, **26**, 4200.

IC-000577

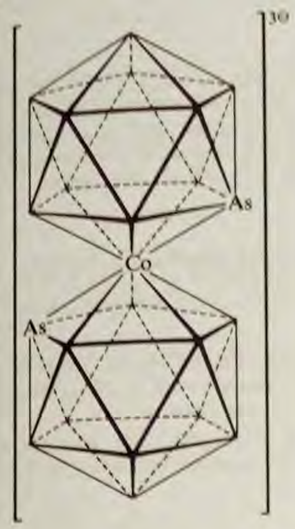
$As_2B_{10}H_{10}$
1,2-Diarsadodecaborane(10), 10CI
[51292-90-1]

M 268.0
Synth. e.g. from decaborane + Et_3N in THF, followed by addn. of $AsCl_3$ in THF and heating under reflux. Off white solid (toluene or C_6H_6). Mp 222-224°.

Little, J.L. *et al*, *Inorg. Chem.*, 1974, **13**, 1752; 1978, **17**, 584 (*synth, ir, pmr, B-11 nmr, derivs*)
Todd, L.J. *et al*, *Inorg. Chem.*, 1987, **26**, 4200 (*synth, derivs*)

IC-000578

$As_2B_{20}CoH_{20}^{3\ominus}$
Bis[(7,8,9,10,11-η)-decahydro-7-arsaundecaborato(2−)] cobaltate(3−)
[65036-28-4]

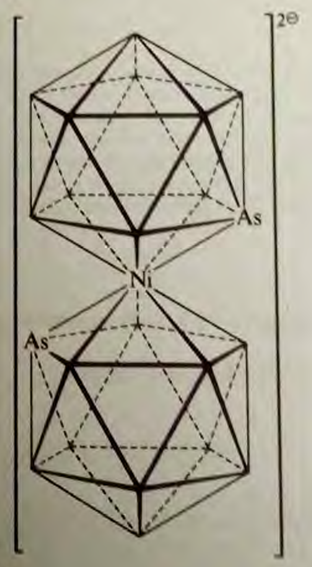


M 445.1 (ion)
Tris-Me_4N salt: [65036-29-5].
Cryst. (hot H_2O). Sol. MeCN.

Little, J.L. *et al*, *Inorg. Chem.*, 1978, **17**, 584 (*synth, ir, pmr, B-11 nmr, uv-vis*)
Geiger, W.E. *et al*, *Inorg. Chem.*, 1982, **21**, 2529 (*elecrochem*)

IC-000579

$As_2B_{20}H_{20}Ni^{2\ominus}$
Bis[(7,8,9,10,11-η)-decahydro-7-arsaundecaborato(2−)] nickelate(2−)



M 444.9 (ion)
Bis-Me_4N salt: [65036-31-9].
Reddish-orange cryst. Sol. MeCN, DMF.

Little, J.L. *et al*, *Inorg. Chem.*, 1978, **17**, 584 (*synth, ir, B-11 nmr, pmr*)

IC-000580

As_2BaZn_2
Barium zinc arsenide ($BaZn_2As_2$)
Barium arsenidozincate(1−) (1:2)
[66540-82-7]

$BaZn_2As_2$

M 417.9
3D struct. with edge and corner shared $ZnAs_4$ tetrahedra with Ba in holes in the network. Synth. from the elements. Orthorhombic cryst.

Klufers, P. *et al*, *Z. Naturforsch., B*, 1978, **33**, 151 (*synth, cryst struct*)

IC-000581

$As_2Br_3Cd_4$
Cadmium arsenide bromide ($Cd_4As_2Br_3$)
[61178-85-6]

$Cd_4As_2Br_3$

M 839.1
Isomorphous with $Cd_4P_2X_3$ (X = Cl, Br or I) and $Cd_4As_2I_3$. Semi-conductor. Dark-red solid.

Suchow, L. *et al*, *J. Electrochem. Soc.*, 1963, **110**, 766 (*synth, powder struct*)
Kikineshi, A.A. *et al*, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, 1984, **27**, 110; *CA*, 1985, **102**, 37849 (*photoelectric effect*)
Gam, N. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1988, **24**, 1574; *CA*, 1989, **110**, 17049 (*photoluminescence, electronic props., photoconduct*)

IC-000582

$As_2Br_3Hg_4$
Mercury arsenide bromide ($Hg_4As_2Br_3$)

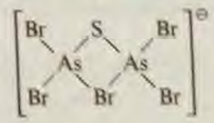
$Hg_4As_2Br_3$

M 1191.9
Isotypic with $Hg_4Sb_2I_3$ etc. Prepd. from As, Hg and Hg_2Br_2. Dark-green solid; slow dec. in daylight; slow dec. in H_2O at 100°; stable in air. Poorly sol. in most solvs.

Puff, H. *et al*, *Z. Anorg. Allg. Chem.*, 1965, **341**, 217 (*synth, powder struct*)

IC-000583

$As_2Br_5S^{\ominus}$
μ-Bromotetrabromo-μ-thioxodiarsenate(*III*)(1−)



M 581.4 (ion)
Ph_4P salt: [102723-46-6].
Synth. from As_2S_3 + Ph_4PBr + HBr(g) in CH_2Br_2. Monoclinic, orange cryst. (cyclohexane). Sol. CH_2Br_2, CH_2Cl_2; insol. toluene, alkanes. The atoms in the anion possess distorted tbp geometry with common edge formed by S and Br atoms. Interatomic distances (mean): As—S 223.9, As—Br (bridge) 283.9, As—Br (terminal) 235.5-249.0 pm: angles: AsBrAs 77.1°, AsSAs 104.9°. Reacts with H_2O → Arsenic sulfide (As_2S_3), IC-000645.

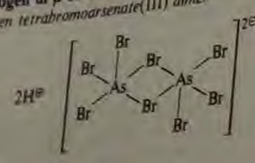
Müller, U. *et al*, *Z. Anorg. Allg. Chem.*, 1986, **533**, 65 (*synth, ir, raman, cryst struct*)

IC-000584

$As_2Br_4H_2$

Dihydrogen di-μ-bromohexabromodiarsenate, 11Cl

Hydrogen tetrabromoarsenate(III) dimer



M 791.0

Bis(N-Methylaniline) salt: [93400-87-4].
Synth. from $AsBr_3$ + PhNHMe in MeCN. Light yellow cryst. Discrete anions with octahedrally coordinated As atoms linked through shared Br atoms. Interatomic distances: As—Br_{term} 234.7, 237.2, 238.7; As—Br_{br} 315.2, 320.3 pm.

Kaub, J. *et al, Z. Naturforsch., B*, 1984, **39**, 1257 (*synth, cryst struct*)

IC-000585

As_2CaMn_2

Calcium manganese arsenide ($CaMn_2As_2$)

$CaMn_2As_2$

M 299.7
Isomorphous with $CaMn_2P_2$. Synth. by heating mixtures of the elements under Ar in a corundum crucible at 900° for 10 h. Crystalline metallic grey black powder; dec. slowly in damp air. Sol. mineral acids. Corresp. Sr and Ba compds. also known.

Mewis, A., *Z. Naturforsch., B*, 1978, **33**, 606 (*synth, props, cryst struct*)
Brunner, E., *Z. Naturforsch., B*, 1978, **33**, 820 (*synth, props, cryst struct*)
Gmelin Handbuch Anorg. Chem., Syst. No. 56, 1983, **C9**, 297 (*rev, bibl*)

IC-000586

As_2CaZn_2

Calcium zinc arsenide ($CaZn_2As_2$)

Calcium arsenidozincate(1−) (1/2)

[62617-34-1]

$CaZn_2As_2$

M 320.7
Struct. resembles $CaAl_2Si_2$. Synth. from the elements. Trigonal cryst.

Klüfers, P. *et al, Z. Naturforsch., B*, 1977, **32**, 353, 753 (*synth, cryst struct*)

IC-000587

$As_2Cd_2O_7$

Cadmium pyroarsenate

Cadmium diarsenate (2-), 11Cl

[68574-20-9]

$Cd_2As_2O_7$

M 486.6
Monoclinic. Synth. from As_2O_5 + CdO at 700°. Dihydrate obt. in the As_2O_5-CdO-H_2O system at 25°. Also synth. by heating $CdAsHO_4$ at 180-200°. Solid.

[66473-70-9]

Bel Kasem Ouanzine, *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **286**, 197 (*synth*)
Nahar, M.A. *et al, Z. Naturforsch., B*, 1978, **33**, 1106 (*synth*)
Juri, M.A. *et al, An. Asoc. Quim. Argent.*, 1981, **69**, 339; *CA*, **96**, 77862 (*synth, ir, cryst struct*)

IC-000588

$As_2Cd_3O_8$

Cadmium arsenate ($Cd_3(AsO_4)_2$)

Cadmium orthoarsenate

[25160-35-4]

$Cd_3(AsO_4)_2$

M 615.0
Prepd. from $CdSO_4$ + Na_2HAsO_4. Cryst. The struct. is similar to that of the mineral graftonite.

Klement, R. *et al, Z. Anorg. Allg. Chem.*, 1964, **334**, 27 (*synth*)
Engel, G. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1970, **132**, 332 (*cryst struct*)

IC-000589

$As_2Cd_4Cl_2$

Cadmium arsenide chloride ($Cd_4As_2Cl_2$)

$Cd_4As_2Cl_2$

M 705.8
Obt. from $CdCl_2$, Cd_3As_2 and As. Deep-red light- and air-stable solid. Isotypic with $Cd_4Sb_2I_2$. Slowly attacked by cold dil. acids and bases.

Puff, H. *et al, Z. Anorg. Allg. Chem.*, 1966, **343**, 259 (*synth, powder struct*)

IC-000590

$As_2Cd_4I_2$

Cadmium arsenide iodide ($Cd_4As_2I_2$)

[57142-92-4]

$Cd_4As_2I_2$

M 980.2
Cd atoms in pseudo cubic face-centred struct.; half As form As—As bonds, which are the shortest bonds in the struct. Semiconductor. Red solid. Isomorphous with $Cd_4As_2Br_2$ and $Cd_4P_2X_2$ (X = Cl, Br or I).

Suchow, L. *et al, J. Electrochem. Soc.*, 1963, **110**, 766 (*synth, optical and electrical props*)
Gallay, J. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2274 (*cryst struct*)
Rebbah, A. *et al, Rev. Chim. Minér.*, 1981, **18**, 125 (*cryst struct*)
Alekseyuk, I.D. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 573 (*synth, ir, thermal anal, powder struct*)
Kikineshi, A.A. *et al, Izv. Vyssh. Uchebn. Zaved., Fiz.*, 1984, **27**, 110; *CA*, 1985, **102**, 37849 (*photoelectric props*)
Gasn, N.S. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1988, **24**, 1574; *CA*, 1989, **110**, 17049 (*photoluminescence, electronic props, photo cond*)

IC-000591

$As_2Cl_4F_6$

Tetrachloroarsenic(1+) hexafluoroarsenate(1−), 9Cl, 8Cl

Tetrachloroarsonium hexafluoroarsenate

[16871-69-5]

$[Cl_4As]^{\oplus}[AsF_6]^{\ominus}$

M 405.6
Tetrahedral cation associated with octahedral anion in solid state. In vapour phase has the covalent struct. Arsenic chloride fluoride ($AsCl_2F_3$), IC-000448. Synth. from $AsCl_3$ + F_2 at −20° or from AsF_3 + Cl_2 at 0°. Colourless, v. hygroscopic cryst. Reacts with Et_2O. Sol. AsF_3 (in which an electrolyte), acetic acid and acetic anhydride. Mp 130° (sealed tube) dec., Mp *ca* 160° (open tube) dec.

Kolditz, L., *Z. Anorg. Allg. Chem.*, 1955, **280**, 313 (*synth, props*)
Weidlein, J. *et al, Z. Anorg. Allg. Chem.*, 1965, **337**, 113 (*synth, ir, raman*)

Preiss, H., *Z. Anorg. Allg. Chem.*, 1971, **380**, 45 (*cryst struct*)
Seppelt, K. *et al, Z. Anorg. Allg. Chem.*, 1978, **439**, 5 (*synth, ir, ms*)
Claus, F. *et al, Z. Anorg. Allg. Chem.*, 1983, **501**, 19 (*synth, ir, ms*)
Elbel, S. *et al, J. Chem. Res. (S)*, 1986, 294 (*pe, ms*)
Minkwitz, R. *et al, Z. Anorg. Allg. Chem.*, 1986, **534**, 150 (*reaction*)

IC-000592

$As_2Cl_4O_3$

Diarsenic tetrachloride trioxide

Diarsenic tetrachloride, 10Cl. Arsenic chloride oxide ($As_2Cl_4O_3$). Pyroarsenic chloride

[60646-37-9]

$[As_2Cl_4O_3]_n$

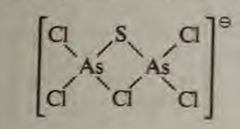
M 339.6
Polymeric; not isostructural with Diphosphoryl chloride, IC-017103. Synth. from $AsCl_3$ + O_3 in $CFCl_3$ at r.t. Stable to 150-200°.

Seppelt, K. *et al, Z. Anorg. Allg. Chem.*, 1978, **439**, 5 (*synth, ir, raman, ms*)

IC-000593

$As_2Cl_5S^{\ominus}$

μ-Chlorotetrachloro-μ-thioxodiarsenate(*III*)(1−), 11Cl



M 359.1 (ion)

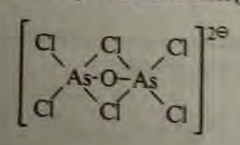
Ph_4P salt: [99021-99-5].
Synth. from As_2S_3 or As_2S_5 + Ph_4PCl + HCl in CH_2Cl_2. Monoclinic pale yellow cryst. Distorted tbp struct. (incl. lone pair) with two pyramids sharing edge between S and Cl. Interatomic distances: As—Cl (bridge) 270.4, As—S 222.7 (mean), As—Cl (terminal) 218.4-230.3 pm; angles: AsSAs 104.0°, AsClAs (bridge) 80.9°.

Mohammed, A.T. *et al, Z. Anorg. Allg. Chem.*, 1985, **523**, 45 (*synth, ir, raman, cryst struct*)

IC-000594

$As_2Cl_6O^{2\ominus}$

Di-μ-chlorotetrachloro-μ-oxodiarsenate(*V*)(2−), 11Cl



M 378.5 (ion)

Di-H compd.: Dihydrogen di-μ-chlorotetrachloro-μ-oxodiarsenate(V)(2−), 11Cl
$As_2Cl_6H_2O$ M 380.5

Bis-pyridinium salt:
$C_{10}H_{12}As_2Cl_6N_2O$ M 538.7
Synth. from $AsCl_3$ + Py.HCl + MeCN aq. Cryst. (MeCN). The two As polyhedra share a Cl,Cl,O face. Interatomic distances: As—Cl 224.2, 226.5 (terminal), 283.6, 296.5 (non-terminal), As—O 176.5 pm.

Kaub, J. *et al, Z. Naturforsch., B*, 1984, **39**, 1252 (*synth, cryst struct*)

IC-000595

$As_2Cl_6S^{2\ominus}$

Di-μ-chlorotetrachloro-μ-thioxodiarsenate(2−), 11Cl

$[As_2Cl_6S]^{2\ominus}$

M 394.6 (ion)

Bis-Ph_4P salt: [95908-46-6].
Synth. from As_2S_3 + $[Ph_4P]Cl$/HCl/1,2-dichloroethane. Colourless needle like cryst. +1 1,2-dichloroethane. Triclinic. Arsenic atoms have distorted octahedral coordination, two octahedra sharing a common face. Lone e.p's are *trans* to sulfur.

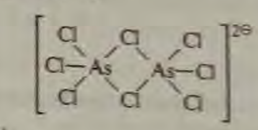
Mohammed, A.T. *et al, Z. Anorg. Allg. Chem.*, 1985, **523**, 45 (*synth, ir, raman, cryst struct*)

IC-000596

$As_2Cl_8^{2\ominus}$

Di-μ-chlorohexachlorodiarsenate(2−), 11Cl

Octachloroarsenate(2−)



M 433.4 (ion)

Bis-Ph_4P salt: Synth. from $AsCl_3$ + Ph_4PCl, or As_2S_3 + Ph_4PCl + HCl in CH_2Cl_2. Pale yellow, rhombic cryst. Triclinic. Anion has two square pyramids sharing basal edge. Interatomic distances: As—Cl (bridge) 274.6, 294.1. As—Cl (terminal) 217.9-230.3 pm; angles: AsClAs (bridge) 98.7°, ClAsCl (ring) 81.3°.

Di-H compd.: see *Dihydrogen di-μ-chlorohexachlorodiarsenate(III)(2−), IC-000597*

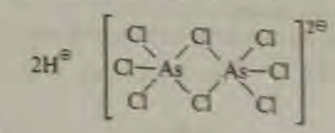
Mohammed, A.T. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 329 (*synth, ir, raman, cryst struct*)
Mohammed, A.T. *et al, Z. Anorg. Allg. Chem.*, 1985, **523**, 45 (*synth*)

IC-000597

$As_2Cl_8H_2$

Dihydrogen di-μ-chlorohexachlorodiarsenate(*III*)(2−), 11Cl

Hydrogen tetrachloroarsenate(III) dimer



M 435.4

Bis-(N-Methylaniline) salt: [93057-60-4].
Synth. from $AsCl_3$ + PhNHMe in HCl (aq.) at r.t. Small colourless leaflets. Discrete anions with pseudo-octahedral coordination for each As atom. Interatomic distances: As—Cl (terminal) 219.7, 221.0, 220.4, As—Cl (bridge) 303.5, 306.3 pm.

Kaub, J. *et al, Z. Naturforsch., B*, 1984, **39**, 1252 (*synth, cryst struct*)

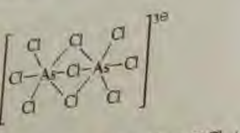
IC-000598

$As_2Cl_8Cs_2$

Tricaesium tri-μ-chlorohexachlorodiarsenate(*III*)(3−), 10Cl

Caesium nonachlorodiarsenate. Caesium enneachlorodiarsenate(III). Caesium chloroarsenate

[71876-08-9]



M 867.6

Hexagonal. As—Cl 225 and 275 pm. Synth. from CsCl + $AsCl_3$. Golden cryst. Dissoc. at 310° to give CsCl + $AsCl_3$.

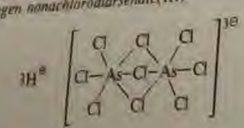
Heard, J.L. *et al*, *J. Chem. Phys.*, 1935, **3**, 117 (*cryst struct*)
Zalewicz, M. *et al*, *Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 1437 (*synth, prop*)

IC-000599

$As_2Cl_4H_3$

Trihydrogen tri-μ-chlorohexachlorodiarsenate(3−)

Trihydrogen nonachlorodiarsenate(III)



M 471.9

Tris-Py salt: [91057-62-6].
$C_{15}H_{18}As_2Cl_9N_3$ M 709.2
Synth. from $AsCl_3$ + Py.HCl in MeCN at r.t. Colourless leaflets + 1MeCN (MeCN). Discrete anions with confacial octahedrally coordinated As atoms. Interatomic distances: As—Cl (bridge) 282.9-308.0; As—Cl (terminal) 221.4-230.0 pm.

Kunk, J. *et al*, *Z. Naturforsch., B*, 1986, **39**, 1252 (*synth, struct*)

IC-000600

$As_2Co_2O_7$

Cobalt(*II*) pyroarsenate

Cobalt(2+) diarsenate (2:1), 1/2/3. Arsenic acid ($H_4As_2O_7$), cobalt(2+) salt (1:2), 8Cl

[26839-15-4]

$Co_2As_2O_7$

M 379.7

Orthorhombic lattice (melanc). Polymorph of the thortveitite struct. Synth. from CoO + As_2O_5 at 600°, or from $CoCl_2$ + $Na_4As_2O_7$. Dark purple solid. Insol. H_2O. Mp ~1125°

Tayne, J.B. *et al*, *Can. J. Chem.*, 1958, **36**, 597 (*synth*)
Ding, J. *et al*, *Can. J. Chem.*, 1970, **48**, 388 (*synth*)

IC-000601

$As_2Cu_3O_8$

Copper arsenate ($Cu_3(AsO_4)_2$)

Copper arsenate (3:2), 1/2/3. Copper(2+) orthoarsenate

[7778-41-8]

$Cu_3(AsO_4)_2$

M 468.4

Polymorphic. In combination with metal chromates, used extensively as a wood preservative.

I-form

Lammerite

Struct. comprises α-PbO_2-type chains of octahedrally coordinated Cu atoms in layers linked by AsO_4 tetrahedra and additional Cu octahedra. Mineral from Bolivia and Namibia. Synth. from As_2O_3 + CuO + H_2O. Monoclinic cryst.

II-form

Two AsO_4 anions have As—O 168 pm and 170 pm. The three cations are 5 coordinated to oxygens. One of Cu's is tbp coordinated. Synth. from Na_2HAsO_4 + $CuCl_2$. Green monoclinic needles or plates.

III-form

Triclinic. Synth. from As_2O_3 + $Cu(NO_3)_2.2H_2O$ + Fe. Emerald green cryst.

[13478-34-7, 54496-60-5]

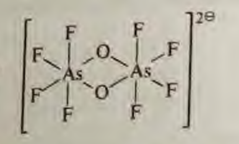
Paulsen, S.J. *et al*, *Can. J. Chem.*, 1968, **46**, 917 (*synth, cryst struct*)
Hawthorne, F.C., *Am. Mineral.*, 1986, **71**, 206 (*mineral*)
Effenberger, H., *Monatsh. Chem.*, 1988, **119**, 1103 (*synth, cryst struct*)

IC-000602

$As_2F_8H_2O_2$

Dihydrogen octafluorodi-μ-oxodiarsenate(*V*)(2−)

[35655-05-1]



M 335.8

Anion possesses the dioxodiarsenate ring struct.

Bis-Py salt: [16962-57-5].
Synth. by heating $K[AsF_4OH]$ at 140°, followed by ion-exchange of the product. White plates. Mp 205-209°. Interatomic distances: As—F 173-181, As—O 181 pm; angle: AsOAs 96°.

Kolditz, L. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **315**, 46; 1965, **335**, 189 (*synth*)
Dunken, H. *et al*, *Z. Chem.*, 1964, **4**, 156 (*cryst struct*)
Haase, W., *Ber. Bunsenges. Phys. Chem.*, 1972, **76**, 1000 (*cryst struct*)
Haase, W., *Chem. Ber.*, 1973, **106**, 734 (*ir, raman*)

IC-000603

$As_2F_{10}K_2O$

Dipotassium decafluoro-μ-oxodiarsenate(*V*)(2−), 8Cl

μ-Oxobispentafluorodiarsenate)

[17653-51-9]

$K_2[F_4AsOAsF_4]$

M 434.0

Monohydrate: [18716-45-5].
Synth. by self-condensation of cobaltocenium salt of $AsF_4OH^{\ominus}$. Orthorhombic cryst. Molecular dimensions: As—O (mean) 173, As—F 171-180 pm.

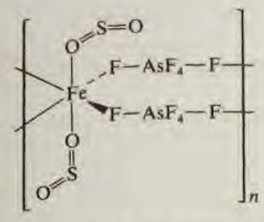
Kolditz, L., *Pure Appl. Chem.*, 1986, **13**, 511 (*rev*)
Kolditz, L. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **354**, 15 (*synth*)
Haase, W., *Ber. Bunsenges. Phys. Chem.*, 1972, **76**, 1000 (*cryst struct*)
Haase, W., *Acta Crystallogr., Sect. B*, 1974, **30**, 1722 (*cryst struct*)

IC-000604

$As_2F_{12}FeO_4S_2$

Bis[hexafluoroarsenato(1−)-*F*]bis(sulfur dioxide-*O*) iron(*II*), 11Cl

[83778-90-9]



M 561.8

Polymeric struct. Should not be formulated as $[Fe(SO_2)_2]^{2\oplus}(AsF_6^{\ominus})_2$. Synth. e.g. by oxidation of Fe using AsF_5 in liq. SO_2 or from $FeBr_2$ + $AgAsF_6$ in liq. SO_2, or from FeF_2 + AsF_5 in liq. SO_2. Sol. liq. SO_2.

Hoppenheit, R. *et al*, *Z. Naturforsch., B*, 1982, **37**, 1116 (*synth, ir, uv, analogue*)

IC-000605

$As_2F_{12}Hg$

Mercury hexafluoroarsenate

Hexafluoroarsenate(1−) mercury(2+) salt (2:1)

[81492-21-9]

$Hg(AsF_6)_2$

M 578.4

Solid. Dec. on heating in Ar with release of AsF_5.

Frlec, B. *et al*, *J. Fluorine Chem.*, 1982, **19**, 485; **20**, 217 (*synth, ir, powder struct, thermal anal*)

IC-000606

$As_2F_{12}Hg_4$

Tetramercury bis-hexafluoroarsenate

[51383-33-6]

$[Hg—Hg—Hg—Hg](AsF_6)_2$

M 1180.1

Contains linear $Hg_4^{2\oplus}$ cations and octahedral $AsF_6^{\ominus}$ anions. Short interactions between cations lead to non-linear chains running through cryst. Synth. from Hg and AsF_5 in SO_2. Red-black needles (SO_2). In soln., is in equil. with $Hg_{2.85}(AsF_6)_2$ and $Hg_3(AsF_6)_2$.

Cutforth, B.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 723 (*synth, cryst struct, raman, uv*)
Cutforth, B.D. *et al*, *Inorg. Chem.*, 1983, **22**, 1344 (*synth, cryst struct*)

IC-000607

$As_2F_{12}Mn$

Manganese(*II*) hexafluoroarsenate

$Mn(AsF_6)_2$

M 432.7

Synth. by reaction of Mn with AsF_5 in liq. SO_2 or liq. HF. Pink cryst. Tetragonal struct.

Clifford, A.F. *et al*, *J. Inorg. Nucl. Chem.*, 1957, **5**, 57 (*synth*)
Dean, P.A.W., *J. Fluorine Chem.*, 1975, **5**, 499 (*synth, magnetism*)
Frlec, B. *et al*, *J. Fluorine Chem.*, 1982, **19**, 485 (*synth, struct, ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, C9, 366 (*rev, bibl*)

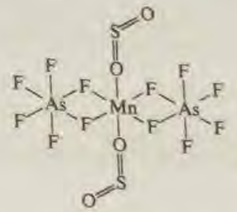
IC-000608

$As_2F_{12}MnO_4S_2$

Bis[hexafluoroarsenato(1−)-*F*]bis(sulfur dioxide-*O*) manganese, 11Cl

Manganese(II) hexafluoroarsenate bis(sulfur dioxide)

[83778-88-5]



M 560.8

Synth. from Mn powder, SO_2 and AsF_5.

Hoppenheit, R. *et al*, *Z. Naturforsch., B*, 1982, **37**, 1116 (*synth, ir, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, C7, 112 (*rev, bibl*)

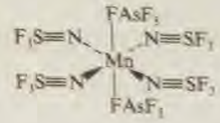
IC-000609

$As_2F_{24}MnN_4S_4$

Bis(hexafluoroarsenato)tetrakis(thiazyltrifluoride) manganese(*II*)

Bis[hexafluoroarsenato(1−)-F]tetrakis(mononitrogen trifluoride monosulfide-N)manganese, 10Cl

[77330-60-0]



M 845.0

Synth. from $Mn(SO_2)_2(AsF_6)_2$ and $N{\equiv}SF_3$. Colourless cryst. (SO_2 or SO_2ClF/SO_2), extremely sensitive to O_2 and moisture. Mp 226°.

[71790-13-1]

Schnepel, F.M. *et al*, *J. Mol. Struct.*, 1980, **60**, 89 (*ir*)
Buss, B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 61 (*synth, ir, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, D7, 220 (*rev, bibl*)

IC-000610

As_2Fe

Iron arsenide ($FeAs_2$)

Arsenoferrite. Iron diarsenide

[12006-21-2]

$FeAs_2$

M 205.6

Has compressed marcasite struct. Obt. by direct combination of elements. Semiconductor (band gap 0.22eV). Source of arsenic. Silver-grey cubic cryst. Insol. H_2O; sl. sol. HNO_3; insol. HCl. Mp 980°. Antiferromagnetic.

Mineral-form [12255-65-1]
Ludlingite. *Loellingite*
Occurs widely in USA, Canada and Europe. Silver-white to steel grey opaque metallic cryst.

Holseth, H. *et al*, *Acta Chem. Scand.*, 1968, **22**, 3273 (*crystal composition*)
Fan, A.K.L. *et al*, *J. Solid State Chem.*, 1972, **5**, 136 (*crystal structure*)

Kjekshus, A. *et al*, *Acta Chem. Scand., Ser. A*, 1974, **28**, 996 (*synth, cryst struct*)
Yuzuri, M. *et al*, *J. Phys. Soc. Jpn.*, 1980, **48**, 1937 (*magnetism, mössbauer*)
Tossell, J.A. *et al*, *Phys. Chem. Miner.*, 1981, **7**, 177 (*electronic struct*)
Burdett, J.K. *et al*, *Inorg. Chem.*, 1982, **21**, 1119 (*struct, electronic struct*)
Lutz, H.D. *et al*, *Phys. Chem. Miner.*, 1983, **9**, 109 (*ir*)
Lutz, H.D. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **554**, 87 (*cryst struct*)

IC-000611

$As_2Fe_2O_8$
Iron(*II*) arsenate ($Fe_2(AsO_4)_2$)
Ferrous arsenate. Iron(II) ortho-*arsenate*
[10102-50-8]

$Fe_2(AsO_4)_2$

M 445.3
Occurs naturally as octahydrate.
▷ NO4580000.
Hexahydrate:
$As_2Fe_2H_{12}O_{14}$ M 553.4
Synth. from $FeSO_4$ + Na_3AsO_4. Insecticide. Green powder. Insol. H_2O; sol. acid. Dec. on heating.
Octahydrate. Symplesite. Parasymplesite
Symplesite is found filling cavities in löllingite, in US, Canada, Germany, Mexico and Morocco.
Parasymplesite occurs in Japan, Morocco, US and Germany. Dimorphic mineral. Indigo blue, light green or light blue powder (Symplesite), or light green- blue cryst. (Parasymplesite).
Gmelin Handbook Inorg. Chem., Syst. No 59, 1931, **B4**, 780 (*rev, bibl*)

IC-000612

$As_2Fe_4O_{11}$
Iron(*III*) arsenate oxide ($Fe_4(AsO_4)_2O_3$)
Angelellite
[12418-53-0]

$Fe_4O_3(AsO_4)_2$

M 549.2
Mineral. Blackish brown.
[12255-71-9]
Ramdohr, P. *et al*, *Am. Mineral.*, 1959, **44**, 1322
Moore, P.B. *et al*, *Neues Jahrb. Mineral., Abh.*, 1978, **132**, 91 (*struct*)

As_2GeO_7 **IC-000613**
Germanium pyroarsenate
Germanium(4+) *diarsenate* (1:1), 9*CI*
[61370-36-3]

$GeAs_2O_7$

M 334.4
Dimorphic. Amorphous form obt. by heating $Ge(HAsO_4)_2$ at 350-430°, product cryst. at 600° → α-$GeAs_2O_7$ which transforms into the β-compd. at 720°. Solid. Dec. at >740° → GeO_2 + As_2O_5 + O_2.
Chernorukov, N.G. *et al*, *Zh. Neorg. Khim.*, 1976, **21**, 2352; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1293 (*synth*)

IC-000614

As_2HO_6P
Arsenic oxide phosphate, 8CI
Arsenic(III) *phosphoric*(V) *oxide* ($2As_2O_3.P_2O_5.H_2O$)
[12429-16-2]

$As_2O_2(HPO_4)$

M 277.8
Synth. from As_2O_3 + H_3PO_4 (aq.). Cryst. Strongly birefringent.
Dachet, J.P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 1767; 1971, **272**, 925 (*synth, cryst struct*)

IC-000615

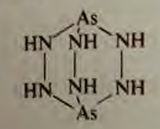
As_2H_4
Diarsine, 9CI, 8CI
Arsinoarsine. Biarsine. Diarsane
[15942-63-9]

H_2AsAsH_2

M 153.8
By product in synth. of AsH_3 by red. of arsenites by borohydrides. Fairly stable gas. Unstable in condensed phase at > −100°.
Saalfield, F.E. *et al*, *Inorg. Chem.*, 1963, **2**, 46, 50 (*synth*)
Saalfield, F.E. *et al*, *Inorg. Chem.*, 1967, **6**, 96 (*ms*)
Gunn, S.R., *Inorg. Chem.*, 1972, **11**, 796 (*props*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 571 (*synth*)

IC-000616

$As_2H_6N_6$
2,3,5,6,7,8-Hexaaza-1,4-diarsa[2.2.2]bicyclooctane
Diarsenic tris(hydrazide)



M 239.9
2,3,5,6,7,8-Hexamethyl. Diarsenic tris(N,N'-*dimethylhydrazide*)
$C_6H_{18}As_2N_6$ M 324.0
Synth. from $As(NMe_2)_3$ + 1,2-dimethylhydrazine. Colourless cryst. V. sol. C_6H_6, toluene, Et_2O, THF; sol. pet. ether. Mp 97-99°.
Nöth, H. *et al*, *Z. Naturforsch., B*, 1965, **20**, 604 (*synth, ir*)

As_2Hg_3 **IC-000617**
Mercury(*II*) arsenide (Hg_3As_2)

Hg_3As_2

M 751.6
Black solid.
▷ Readily oxidised, spontaneously flammable when dry.
Brukl, A., *Z. Anorg. Allg. Chem.*, 1923, **131**, 236 (*synth*)

$As_2Hg_3O_8$ **IC-000618**
Mercury(*II*) arsenate ($Hg_3(AsO_4)_2$)
Mercuric orthoarsenate
[13437-80-4]

$Hg_3(AsO_4)_2$

M 879.6

Obt. from the As_2O_5—HgO—H_2O system. Yellow microcryst. needles. Pract. insol. H_2O. Mp 575° dec.
Guerin, H. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1950, **230**, 447; 1951, **232**, 65 (*synth*)

IC-000619

$As_2Hg_4I_2$
Mercury arsenide iodide ($Hg_4As_2I_2$)
[12255-76-4]

$Hg_4As_2I_2$

M 1332.9
Struct. is described as either a pseudo-cubic close packing of Hg atoms with As and I in the interstices or a complex arrangement of two polyhedra surrounding Hg, sharing edges or corners. Short As—As bonds in the solid state. Isostructural with $Cd_4As_2I_2$. Prepd. from As, Hg and Hg_2I_2. Black cryst. Semiconductor. Resistant to non-oxidising acids. Slow dec. in H_2O at 100°.
Puff, H. *et al*, *Z. Anorg. Allg. Chem.*, 1965, **341**, 217 (*powder struct, synth*)
Labbé, P.L. *et al*, *Z. Kristallogr.*, 1989, **187**, 117 (*synth, cryst struct*)

IC-000620

As_2I_4
Arsenic iodide (As_2I_4), 10CI
Diarsenic(III) *tetraiodide. Tetraiododiarsenic*(III)
[13770-56-4]

I_2AsAsI_2

M 657.4
Synth. from As or AsI_3 + I_2 at 240-260° in sealed tube. Red cryst. Stable in inert atm. to 150°. Readily dec. by air or H_2O. Disproportionates on heating becoming quantitative at 400°. Mp 137°.
Chernov, A.P. *et al*, *Zh. Neorg. Khim.*, 1973, **18**, 2876; *Russ. J Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 1530 (*props, form*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 575 (*synth*)
Bastow, J.J. *et al*, *J. Magn. Reson.*, 1980, **37**, 269 (*synth, nqr*)

$As_2MnS_5Tl_2$ **IC-000621**
Manganese thallium arsenide sulfide ($MnTl_2As_2S_5$)

$MnTl_2As_2S_5$

M 773.8
Shows orthorhombic symmetry. The Tl is surrounded irregularly by 6 S atoms, Mn comprises sl. distorted MnS_6 octahedra, and the As atom has trigonal pyramidal coordination with 3 S atoms. Forms between 230-260° at 5-18 atm. under hydrothermal conditions. Dark brown cryst.; thin sections are red in transmitted light.
Gostojić, M. *et al*, *Z. Kristallogr.*, 1982, **158**, 43 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 369 (*rev, bibl*)

As_2MnSe_4 **IC-000622**
Manganese arsenide selenide ($MnAs_2Se_4$)

$MnAs_2Se_4$

M 520.6
Tetragonal struct. Formed in the MnSe-As_2Se_3 system at 750-800° $Mn_3As_2Se_8$ also known. *p*-type semiconductor. Solid, stable to air and H_2O. Mp 420° (congr.).
Rustamov, P.G. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 84 (*synth, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 372 (*rev, bibl*)

As_2MnTe_4 **IC-000623**
Manganese arsenide telluride ($MnAs_2Te_4$)

$MnAs_2Te_4$

M 715.1
Tetragonal struct. Formed in the MnTe-As_2Te_3 system. $Mn_3As_2Te_6$ also known. Mp 605° (congr.).
Rustamov, P.G. *et al*, *CA*, 1979, **91**, 45097 (*prop, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 374 (*rev, bibl*)

$As_2Mn_2O_7$ **IC-000624**
Manganese(*II*) pyroarsenate
Manganese(2+) *diarsenate* (2:1), 9*CI*
[58593-68-3]

$Mn_2As_2O_7$

M 371.7
Obt. by heating $MnHAsO_4.H_2O$ at ca. 200°; $Mn(NH_4)AsO_4.H_2O$ at 800°; or As_2O_5 + $MnCO_3$ at 600°. Monoclinic lattice.
Botto, I.L., *Monatsh. Chem.*, 1975, **106**, 1559 (*synth, ir, cryst struct*)
Nabar, M.A. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1106 (*synth*)

$As_2Mn_3O_8$ **IC-000625**
Manganese(*II*) arsenate(*V*) ($Mn_3(AsO_4)_2$)

$Mn_3(AsO_4)_2$

M 442.6
The existence of anhydrous $Mn_3(AsO_4)_2$ is doubtful. The monohydrate is present in the $Mn_3(AsO_4)_2$—H_3AsO_4—H_2O system. The tetrahydrate is only known as the mineral.
Monohydrate:
$As_2H_2Mn_3O_9$ M 460.6
Synth. by reaction of aq. solns. of Na_3AsO_4 and $MnSO_4$ in a closed tube at *ca.* 175°. Maroon needles.
Tetrahydrate: [77171-60-9]. ***Sterlinghillite***
$As_2H_8Mn_3O_{12}$ M 514.7
Light pink cryst.
Ephraim, F. *et al*, *Helv. Chim. Acta*, 1929, **12**, 1025 (*synth, monohydrate*)
Dunn, P.J., *Am. Mineral.*, 1981, **66**, 182 (*struct, tetrahydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 325 (*rev, bibl*)

$As_2Na_4O_7$ **IC-000626**
Tetrasodium diarsenate, 9CI
Sodium diarsenate ($Na_4As_2O_7$). *Sodium pyroarsenate. Tetrasodium pyroarsenate*
[13464-42-1]

$Na_4As_2O_7$

M 353.7
Monoclinic. Anion consists of two AsO_4 tetrahedra sharing a common O with bridging angle AsOAs 123.5°, and bridge As—O 178.3 pm. Terminal As—O 165.8 pm. By dehydration of Na_2HAsO_4 at 130-900°, or from

$Na_3AsO_4 + As_2O_5$ at melt. Colourless cryst. Readily sol. H_2O. Mp 848°. A reversible structure phase change is observable at 692°. Dec. > 700° → Pentasodium triarsenate, IC-000659.

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 947; Suppl. Vol., 1967, 4, 1700 (rev, bibl)
Stec, W.J. *et al, Inorg. Chem.*, 1972, **11**, 219 (*pe*)
Leung, K.Y. *et al, Can. J. Chem.*, 1973, **51**, 2082 (*synth, cryst struct*)
Donski, K. *et al, Collect. Czech. Chem. Commun.*, 1973, **38**, 667 (*synth*)
Beilins, A.Z. *et al, Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 148 (*ir, raman*)
Drábová, M. *et al, Collect. Czech. Chem. Commun.*, 1987, **52**, 1488 (*synth*)

IC-000627

As_2O_5

Arsenic oxide (As_2O_5), 9CI, 8CI

Diarsenic trioxide. Arsenious oxide. Arsenic sesquioxide. White arsenic. Arsenous acid anhydride. Arsenous oxide

[1327-53-3]

As_2O_5

M 197.8

Formed on burning As in air, or from $AsCl_3 + H_2O$; from arsenopyrites by roasting. Also by heating Arsenic oxide (As_4O_6), IC-000665 (arsenolite) at 100-200° or higher temp. in absence of H_2O. Probably the most important compound of arsenic. Used in optical glasses and glasses for electronic equipment. Acts as a wood preservative. Occurs as air pollutant from metal smelting plants and power plants. Commercially available. White powder. Sol. H_2O (2.16 g per 100 cm^3 at 25°). Mp 312°. In vap., exists as Arsenic oxide (As_4O_6), IC-000665. With PCl_5 or $POCl_3$ → $AsCl_3$.

▷ Highly toxic. Carcinogenic. Inflames in contact with $NaClO_3$. CG3325000.

Mineral-form [13473-03-5]

Claudetite

Exists in two forms, both monoclinic, differing in arrangement of As atoms placed between puckered layers of oxygen atoms. The mean shorter As—O distances are 177.2 pm (Claudetite I) and 179 pm (Claudetite II).

Dimer: see Arsenic oxide (As_4O_6), IC-000665
Gmelin Handbook Inorg. Chem., Syst. No. 17, 1932, 236 (rev, bibl)
Becker, K.A. *et al, Prog. Inorg. Chem.*, 1962, **4**, 1 (*rev, bibl*)
Ban, V.S. *et al, J. Chem. Phys.*, 1970, **52**, 248 (*ms*)
Pertlik, F., *Monatsh. Chem.*, 1975, **106**, 755; 1978, **109**, 277 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, I, 580 (*synth*)
Hyun, E.J. *et al, Phys. Rev. B: Solid State*, 1976, **13**, 1752 (*ir, raman*)
Leonhardt, G. *et al, Phys. Ser.*, 1977, **16**, 448 (*pe*)
Wimmer, E. *et al, Phys. Status Solidi B*, 1978, **89**, 619 (*pe*)
Mercier, R. *et al, Spectrochim. Acta, Part A*, 1978, **34**, 337 (*ir, raman*)
Treacy, D.J. *et al, Solid State Commun.*, 1981, **40**, 135 (*nqr*)
Brittain, R.D. *et al, J. Phys. Chem.*, 1982, **86**, 5072 (*ms*)
Voigt, B. *et al, Monatsh. Chem.*, 1982, **113**, 895.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 305.

As_2O_4

Arsenic oxide (As_2O_4), 10Cl, 8Cl IC-000628

Diarsenic tetroxide

[12505-65-6]

As_2O_4

M 213.8

Orthorhombic. Infinite layer struct. containing As(*III*) (tbp) and As(*V*) (tetrahedral) coordinated groups. Synth. from As_2O_3 + As_2O_5, heated in the presence of water → 6:5 hydrate. Solid, stable at 400°.

Hydrate (6:5): $As_{12}H_{10}O_{29}$.
Solid, stable at 110°.

Long, L.H. *et al, J. Inorg. Nucl. Chem.*, 1963, **25**, 79 (*synth*)
Jones, P.G. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 439 (*cryst struct*)
Barten, H. *et al, Thermochim. Acta*, 1984, **78**, 431 (*props*)

As_2O_4Pb

Lead metaarsenite ($Pb(AsO_2)_2$) IC-000629

[10031-13-7]

$Pb(AsO_2)_2$

M 421.0

White cryst. powder. Insol. cold H_2O; sol. HNO_3.

▷ Toxic. OF8600000.

U.S. Pat., 4 152 280, (1979); *CA*, **91**, 61703 (*use*)

As_2O_5

Arsenic oxide (As_2O_5), 9CI, 8CI IC-000630

Diarsenic(V) pentoxide. Arsenic pentoxide (incorr.)

[1303-28-2]

As_2O_5

M 229.8

Struct. formed by corner sharing of AsO_6 octahedra and AsO_4 tetrahedra with As—O 181.8 and 167.6 pm resp. Synth. from As_2O_3 + c. HNO_3, 3:5 hydrate heated at > 170°. Oxidation catalyst (e.g. in heterocyclic synth.). Wood preservative. Commercially available. Deliquescent solid. V. sol. H_2O (230 g per 100 cm^3 at 20°). Shows phase change at 225° to high temp. tetragonal form. For molecular form, As_4O_{10}, see under Arsenic oxide (As_4O_6), IC-000665.

▷ Poison. CG2275000.

Hydrate (3:5): see Triarsenic acid, IC-000656
Tetrahydrate: see Arsenic acid, IC-000500
Heptahydrate: see Arsenic acid, IC-000500
Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 273 (rev, bibl)
Stec, W.J. *et al, Inorg. Chem.*, 1972, **11**, 219 (*pe*)
Jansen, M., *Z. Anorg. Allg. Chem.*, 1978, **441**, 5 (*synth, cryst struct*)
Barton, H., *J. Appl. Chem.*, 1981, **14**, 68 (*synth, cryst struct*)
Plies, V. *et al, Z. Anorg. Allg. Chem.*, 1983, **497**, 185 (*ms*)
Jansen, M., *Nova Acta Leopold*, 1985, **59**, 121 (*rev. bibl*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 304.

As_2O_6Pb

Lead diarsenate(*V*) IC-000631

Lead arsenate ($PbAs_2O_6$). Lead(II) metaarsenate(V)

[13464-43-2]

$PbAs_2O_6$

M 453.0

Hexagonal tablets or transparent glass. Sol. HNO_3. Dec. in H_2O. Glass absorbs moisture rapidly, becoming opaque.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 195.
Gmelin Handbook Inorg. Chem., Syst. No. 47, 1970, C3, 898 (bibl)
Nakhmetov, M.Zh. *et al, Term. Anal., Tezisy Dokl. Vses. Soveshch., 7th, 1979*, 7th, 1979, **1**, 157 (*synth*)
Shigematsu, K. *et al, Nippon Kogyo Kaishi*, 1982, **98**, 611 (*ir*)

$As_2O_7Pb_2$

Lead pyroarsenate ($Pb_2As_2O_7$) IC-000632

Lead(II) diarsenate(V)

[13510-94-6]

$Pb_2As_2O_7$

M 676.2

Rhombic yellow cryst. Insol. cold H_2O, insol. acids. Mp 802°. Dec. in hot H_2O.

McDonnell, C.C. *et al, J. Am. Chem. Soc.*, 1916, **18**, 2027 (*synth, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 47, 1970, C3, 898 (rev, bibl)
Nabov, M.A. *et al, J. Appl. Crystallogr.*, 1978, **11**, 162 (*cryst struct*)
Makhmetov, M.Zh. *et al, Tezisy. Dokl.- Vses. Konf. Khim. Soveshch.*, 1979, **1**, 157; *CA*, **93**, 214708f (*synth*)

$As_2O_7Sn_2$

Tin pyroarsenate ($Sn_2(As_2O_7)$) IC-000633

Ditin pyroarsenate

$Sn_2As_2O_7$

M 499.2

Flocculent solid. Insol. H_2O, insol. conc. HOAc. Dec. to $As_2O_5 + SnO_2$.

Prasad, A. *et al, Proc. - Indian Acad. Sci., Sect. A*, 1943, **17**, 161.

$As_2O_8Pb_3$

Lead arsenate ($Pb_3(AsO_4)_2$) IC-000634

Lead orthoarsenate ($Pb_3(AsO_4)_2$)

[3687-31-8]

$Pb_3(AsO_4)_2$

M 899.4

Double layer struct: 2 sheets of AsO_4 tetrahedra with Pb atoms in between. Another group of Pb atoms lies in the same plane as O. Yellow-white or white cryst. V. sl. sol. cold H_2O; sol. HNO_3. Mp 1042°. Sl. dec. at 1000°.

▷ V. poisonous. CG0990000.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 191 (*bibl*)
Gerlach, J. *et al, Metall (Berlin)*, 1968, **22**, 812 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 47, 1970, C3, 894 (rev, bibl)
Viswanathan, K. *et al, Z. Kristallogr.*, 1978, **148**, 275 (*cryst struct*)
Nakhmetov, M.Zh. *et al, Term. Anal., Tezisy Dokl. Vses. Soveshch., 7th, 1979*, 7th, 1979, **1**, 157 (*synth*)

$As_2O_8Zn_3$

Zinc arsenate ($Zn_3(AsO_4)_2$) IC-000635

[13464-44-3]

$Zn_3(AsO_4)_2$

M 474.0

Prepd. by reaction of $ZnSO_4$ with Na_2HAsO_4. Wood preservative.

Octahydrate: [16484-91-6]. ***Kottigite.*** *Koettigite*
Mineral. Insol. H_2O.

Klement, R. *et al, Z. Anorg. Allg. Chem.*, 1964, **334**, 27 (*synth*)
Sturman, B.D., *Can. Mineral.*, 1976, **14**, 437 (*mineral*)
Hill, R.J. *et al, Am. Mineral.*, 1979, **64**, 376 (*cryst struct, kottigite*)

$As_2O_{11}Ti_3$

Titanium arsenate oxide ($Ti_3(AsO_4)_2O_3$) IC-000636

Bis[tetraoxoarsenato(3−)]trioxotrititaniate(1V), 11Cl

[62712-27-0]

$Ti_3O_3(AsO_4)_2$

M 469.4

Synth. by heating $TiO_2 + As_2O_5$; the compd. is also formed in the precipation of arsenic from electrolysis solns. with $(NH_4)_2TiO(SO_4)_2$ at 50-80°. Mp 940° dec.

Baipeisova, B.S. *et al, CA*, 1979, **91**, 125432c (*synth*)
Baipeisova, B.S. *et al, CA*, 1980, **93**, 81409k (*synth*)
Buketov, E.A. *et al, Vestn. Akad. Nauk Kaz. SSR*, 1982, 49; *CA*, **97**, 173936r (*synth from $TiO_2 + As_2O_5$*)

$As_2O_{12}S_3$

Arsenic(*III*) sulfate IC-000637

Arsenous sulfate

[65496-42-6]

$As_2(SO_4)_3$

M 438.0

Monoclinic cryst. Each SO_4 group bridges two AsO_3 pyramids. Interatomic: distances S—O 154, As—O 183, S=O 142 pm. Synth. from As_2O_3 + oleum at 70°. V hygroscopic cryst.

Douglade, J. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 720 (*synth, raman, cryst struct*)

$As_2O_{62}W_{18}^{7\ominus}$

Tungstoarsenate ($As_2W_{18}O_{62}^{7\ominus}$), 8Cl IC-000638

Bis[orthoarsenato(3−)]tetrapentacontaoxooctadecatungstate(7−), 10Cl

[59965-04-7]

$[As_2W_{18}O_{62}]^{7\ominus}$

M 4451.1 (ion)

Heteropolyanion. Formed in soln. by electrochem. reduction of $[As_2W_{18}O_{62}]^{6\ominus}$.

Prados, R.A. *et al, Inorg. Chem.*, 1976, **15**, 2547 (*formn, esr*)
Sanchez, C. *et al, J. Am. Chem. Soc.*, 1983, **105**, 6817 (*formn, esr*)

$As_2O_{62}W_{18}^{6\ominus}$

Tungstoarsenate ($As_2W_{18}O_{62}^{6\ominus}$), 8Cl IC-000639

Bis[μ_9-[orthoarsenato(3−)]]hexatriaconta-μ-oxooctadecaoxooctadecatungstate(6−), 10Cl

[12267-69-5]

$[As_2W_{18}O_{62}]^{6\ominus}$

M 4451.1 (ion)

At least 2 isomeric forms are known. Prepared by heating solns. of As_2O_5 + $[WO_4]^{2\ominus}$.

Hexa-NH_4 salt: [89655-89-0].
Lemon-yellow cryst. (H_2O) or orange cryst.

[37365-59-6, 89675-80-9, 89689-31-6, 112570-96-4, 113477-89-7]

Acerete, R. *et al, Inorg. Chem.*, 1984, **23**, 1478 (*synth, IR-183 nmr, isom*)
Neubart, H. *et al, Z. Naturforsch., B*, 1987, **42**, 951 (*cryst struct, isom*)

$As_2O_{68}W_{20}^{10\ominus}$

Tungstoarsenate ($As_2W_{20}O_{68}^{10\ominus}$), 8Cl IC-000640

Bis[μ_9-[arsenito(3−)]]octatriaconta-μ-oxotetracosaoxoicosatungstate(10−), 10Cl

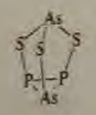
$[As_2W_3O_{10}]^{n\ominus}$

M 4914.8 (min)
Heteropolyanion. May be $[As_2W_3O_{10}(H_2O)]^{n\ominus}$. Prepd. by base hydrol. of $[As_2W_{21}O_{69}]^{6\ominus}$
Deca-K salt: [88289-49-0]
Cryst.
Leyrie, M. *et al. Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **279**, 895 (*synth*)
Lefebvre, F. *et al. Inorg. Chim. Acta*, 1983, **73**, 173 (*synth, ir*)

IC-000641

$As_2P_2S_3$

Arsenic phosphorus sulfide ($As_2P_2S_3$)
3,5,7-Trithia-1,2-diphospha-4,6-diarsatricyclo[2.2.1.0^{2,6}]heptane, 1ICI
[92477-60-6]



M 307.9
Synth. from P_4S_3 + As_4S_3. Orthorhombic.
Blachnik, R. *et al. Z. Naturforsch., B*, 1984, **39**, 1135 (*P-31 nmr*)
Christian, B.H. *et al. Acta Crystallogr., Sect. C*, 1987, **43**, 187 (*cryst struct*)
Baldus, H.P. *et al. Monatsh. Chem.*, 1988, **119**, 515 (*synth, purif*)

IC-000642

$As_2P_2S_3$

Arsenic phosphorus sulfide ($As_2P_2S_3$)
3,5,7-Trithia-1,4-diphospha-2,6-diarsatricyclo[2.2.1.0^{2,6}]heptane, 1ICI
[54321-45-8]

M 307.9
In molten state, in equilibrium with Arsenic phosphorus sulfide (As_6PS_3), IC-000660 and Arsenic sulfide (As_4S_4), IC-000666. Yellow needles (CS_2) which melt to red liq. Insol. most org. solvs. Sol. CS_2. Mp 228-230°.
Leva, A.M. *et al. Z. Anorg. Allg. Chem.*, 1974, **409**, 215 (*synth, ir, raman, props*)
Blachnik, R. *et al. Z. Naturforsch., B*, 1981, **36**, 1493; 1984, **39**, 1135 (*P-31 nmr, ms*)
Buss, W. *et al. Z. Anorg. Allg. Chem.*, 1984, **516**, 42 (*formn*)
Operti, L. *et al. Inorg. Chim. Acta*, 1985, **98**, 43 (*ms*)
Christian, B.H. *et al. Acta Crystallogr., Sect. C*, 1987, **43**, 187 (*cryst struct*)

$As_2P_2S_5$

IC-000643

Arsenic phosphorus sulfide ($As_2P_2S_5$), 1ICl
Arsenic thiodiphosphate, 1ICI 2,6-Epithio[1,3,2,4,5]dithiazaphosphadiarsole[4,5-d][1,3,2,4,5]dithiazaphosphadiarsole 2,6-disulfide
[79278-21-0]

M 436.2
Interatomic distances: As—As 250.9, As—S 225.7, P—S 208.3, P=S 193.2 pm. Synth. from As + S at 350°
Light yellow needles.
Wibbelmann, C. *et al. Z. Naturforsch., A*, 1981, **36**, 836 (*synth, ir, raman, ms, struct*)
Cyvin, S.J. *et al. Z. Naturforsch., A*, 1983, **38**, 987 (*struct*)
Hönle, W. *et al. Z. Naturforsch., B*, 1984, **39**, 1088 (*synth, cryst struct*)

IC-000644

As_2Pt

Platinum arsenide ($PtAs_2$), 9CI
[12044-52-9]

$PtAs_2$

M 344.9
Has iron pyrites struct. Synth. from Platinum, IC-021805 + As. Dull grey solid. Dec. above 800°.
▷ Synth. possibly hazardous.

Mineral-form

Sperrylite
Member of pyrite group. Occurs widely. A principal source of Pt. Metallic white cryst.

Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1625.
Wells, A.F., *Structural Inorg. Chem.*, 5th Ed. Oxford, 1984, 760 (*struct*)
Lutz, H.D. *et al. J. Phys. Chem. Solids*, 1985, **46**, 437 (*ir*)

IC-000645

As_2S_3

Arsenic sulfide (As_2S_3), 9CI, 8CI
Arsenic(III) sulfide. Diarsenic trisulfide. Arsenic sesquisulfide
[1303-33-9]

As_2S_3

M 246.0
Exists in amorphous and vitreous states as well as cryst. Latter is monoclinic with a layer struct. (*cf.* As_2O_3) with each As bonded pyramidally to 3 × S at 224 pm. From As + S at high temp. in sealed ampoule; from As_2O_3 + S; in colloidal form from $As^{3\oplus}$ + H_2S at pH 1-2. Pigment: identified in mediaeval manuscripts (eg. from Armenia). Semiconductor. Used in optical materials, eg. antireflective layers. Photoconductive and used in hologram recording. Commercially available. Red needles or yellow in polycryst. form. Insol. H_2O. Mp 327° (310°). Bp 710° (extrap.). Sublimes readily below Mp. Vap. consists of As_4S_6 molecules (*cf.* As_4O_6). Burns when heated in air → As_2O_3 + SO_2. Cl_2 → $AsCl_3$ + S_2Cl_2. Dissolves readily in $OH^\ominus$ aq. Boiling Na_2CO_3 soln. → Arsenic sulfide (As_4S_4). IC-000668.
▷ Poison. Carcinogen. CG2638000.

Mineral-form

Orpiment: Yellow arsenic sulfide. Arsenic yellow. King's yellow. C.I. 77086
Occurs in lignite (Czechoslovakia), gold ores (Nevada, U.S.A.; Armenia), hot springs (Japan, and Kamchatka, U.S.S.R.) as well as in Switzerland, Yugoslavia. Yellow solid.

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 422 (*rev, bibl*)
Dembovskii, S.A. *et al. Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 787; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 669 (*comb, cryst struct*)
Kravchenko, E.A. *et al. Phys. Status Solidi*, 1969, **31**, K19 (*npr*)
Mathieu, J.-P. *Bull. Soc. Fr. Mineral. Cristallogr.*, 1970, **93**, 532 (*ir, raman*)
Bue, V.S. *et al. J. Chem. Phys.*, 1970, **52**, 248 (*mol*)

Vaipolin, A.A., *Zh. Strukt. Khim.*, 1970, **11**, 484; *J. Struct. Chem. USSR (Engl. Transl.)*, 1970, **11**, 443 (*rev*)
Koblinska, R.J. *et al. Phys. Rev. B: Solid State*, 1973, **8**, 756 (*ir, raman*)
Poltavtsev, Yu.G., *Zh. Fiz. Khim.*, 1975, **49**, 1689, 1692; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1975, **49**, 996, 998 (*struct*)
Nabitovich, I.-D. *et al. Kristallografiya*, 1976, **21**, 620; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1976, **21**, 348 (*struct, ed*)
Seregin, P.P. *et al. Fiz. Khim. Steckla*, 1977, **3**, 512; *Sov. J. Glass Phys. Chem. (Engl. Transl.)*, 1977, **3**, 470 (*pe*)
Bertoluzza, A. *et al. J. Non-Cryst. Solids*, 1978, **29**, 49 (*ir, raman*)
Wimmer, E. *et al. Phys. Status Solidi B*, 1978, **89**, 619 (*pe*)
Voigt, B. *et al. Monatsh. Chem.*, 1982, **113**, 895 (*synth*)
Audrieth, A.M., *J. Non-Cryst. Solids*, 1985, **77-78**, 1219 (*optical and photoelectric props, rev*)
Mills, G. *et al. J. Phys. Chem.*, 1988, **92**, 822 (*synth, props*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 304.

IC-000646

As_2S_5

Arsenic sulfide (As_2S_5), 9CI, 8CI
Diarsenic pentasulfide. Arsenic pentasulfide (incorr.). Arsenic(V) sulfide
[1303-34-0]

As_2S_5

M 310.1
Exists in crystalline and vitreous forms. Synth. by reaction of orthoarsenate solns. + H_2S; or Na_3AsS_4 aq. + $H^\oplus$. Employed in photoimagery. Acoustooptic modulator material. Yellow solid. Dec. in air at *ca.* 95° → S + Arsenic sulfide (As_2S_3), IC-000645. Boiling H_2O → As_2O_3 + S + As_2S_3. Dissolves in solns. of metallic (eg. Gp. I) sulfides giving thioarsenates.
▷ Flammable as dust; explosive with powerful oxidants.

Vaipolin, A.A. *et al, Fiz. Tverd. Tela (Leningrad)*, 1963, **5**, 683; *Soviet Phys.: Solid State (Engl. Transl.)*, 1963, **5**, 497 (*struct*)
Timofeeva, N.V. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1970, **190**, 902; *Dokl. Phys. Chem. (Engl. Transl.)*, 1970, **190**, 115 (*cryst struct*)
Thilo, E. *et al, Z. Anorg. Allg. Chem.*, 1970, **373**, 111 (*synth*)
Stec, W.J. *et al, Inorg. Chem.*, 1972, **11**, 219 (*pe*)
Poltavtsev, Yu.G., *Zh. Fiz. Khim.*, 1975, **49**, 1425; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1975, **49**, 840 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 582 (*synth*)
Diemann, E., *Rev. Chim. Minér.*, 1979, **16**, 237 (*synth, ir, raman, uv, pe*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 304 (*haz, toxicity*)

IC-000647

As_2SeTe_2

Arsenic selenide telluride (As_2SeTe_2), 9CI, 8CI
[12255-92-4]

As_2SeTe_2 or $As_2Se_3.2As_2Te_3$

M 484.0
Exists in vitreous and cryst. forms. Synth. from elements. Possesses piezoelectric props. Solid. Mp 323-344°.

Edmond, J.T., *Brit. J. Appl. Phys.*, 1966, **17**, 979 (*electrical, optical props*)
Bagley, B.G. *et al, J. Non-Cryst. Solids*, 1970, **2**, 155, 161 (*props*)
Voivodov, E. *et al. J. Non-Cryst. Solids*, 1974, **15**, 275 (*props*)
Chang, J. *et al, J. Non-Cryst. Solids*, 1974, **16**, 72 (*rel*)

IC-000648

As_2Se_2Te

Arsenic selenide telluride (As_2Se_2Te), 9CI, 8CI
[12255-93-5]

As_2Se_2Te or $2As_2Se_3.As_2Te_3$

M 435.3
Does not cryst. Synth. from elements. Solid. Vitreous, softening at 155-160°.
Edmond, J.T., *Brit. J. Appl. Phys.*, 1966, **17**, 979 (*electrical, optical props*)
Bagley, B.G. *et al, J. Non-Cryst. Solids*, 1970, **2**, 155, 161 (*props*)
Chang, J. *et al, J. Non-Cryst. Solids*, 1974, **16**, 72 (*rel*)
Banëk, I., *Czech. J. Phys. (Engl. Transl.)*, 1975, **B25**, 1319 (*electrical props*)

As_2Se_3

Arsenic selenide (As_2Se_3), 9CI, 8CI IC-000649
Diarsenic(III) triselenide. Selenium arsenide. Arsenic sesquiselenide
[1303-36-2]

As_2Se_3

M 386.7
Monoclinic. In cryst. each As atom is surrounded by polyhedron of 7 Se atoms forming distorted tetragonal pyramid and triangular prism, one face of which coincides with base of pyr. Mean As—Se 240 pm. Also known in amorphous and vitreous forms. From As_4Se_4 at 260°; annealing of vitreous form at 320°; As + Se heated *in vacuo* → amorphous form. Photoconductor and important xerographic photoreceptor, props. better than those of Se itself. Semiconductor. Used in glass optical fibres. Commercially available. Cherry red cryst. Mp 380° (370°). Bp 861° (extrap.) (846°).

Vitreous-form

Trigonal struct. Stable, brown, semi-conducting glass. Cryst. at 280° after softening at *ca.* 180-187°. ΔH°_{298} − 122 kJ.

Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 463 (*rev, bibl*)
Myers, M.B. *et al, Mater. Res. Bull.*, 1967, **2**, 535 (*synth, phase diagram*)
Kravchenko, E.A. *et al, Phys. Status Solidi*, 1969, **31**, K19 (*npr*)
Whitfield, H.J., *Aust. J. Chem.*, 1971, **24**, 697 (*synth, ir*)
Renninger, A.L. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 1583 (*cryst struct*)
Zakharov, V.P. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1973, **9**, 891; *Inorg. Materials (Engl. Transl.)*, 1973, **9**, 791 (*synth, ir*)
Baker, E.H., *J. Chem. Soc., Dalton Trans.*, 1975, 1589 (*synth, props*)
Arai, T. *et al, J. Non-Cryst. Solids*, 1975, **18**, 289 (*vib spectra*)
Nabitovich, I.D. *et al, Kristallografiya*, 1976, **21**, 620; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1976, **21**, 348 (*rel*)
Strom, U. *et al, Phys. Rev. B: Solid State*, 1977, **16**, 5512 (*ir, microwave*)
Bahl, M.K. *et al, J. Chem. Phys.*, 1980, **72**, 4069 (*pe, auger*)
Gosh, B. *et al, Prog. Cryst. Growth Charact.*, 1983, **6**, 393 (*cryst, props, rev*)
Freitas, J.A. *et al, J. Non-Cryst. Solids*, 1985, **77-78**, 1125 (*raman*)
Stergiou, A.C. *et al, Z. Kristallogr.*, 1985, **173**, 185 (*comb, cryst struct*)
Antonelli, A. *et al, Phys. Rev. B: Solid State*, 1986, **33**, 2968 (*struct*)
Tarnow, E. *et al, Phys. Rev. B: Solid State*, 1988, **38**, 4059 (*struct*)
Neverov, V.G. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1989, **25**, 225; *Inorg. Materials (Engl. Transl.)*, 1989, **25**, 191

IC-000650

As_2Si

Silicon arsenide ($SiAs_2$)
Silicon diarsenide
[12255-97-9]

$SiAs_2$

M 177.9
Semiconductor. Cryst.

Danashevskaya, E.P. *et al*, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, 1974, **17**, 142.
Wadsten, T., *Chem. Comm. Univ. Stockholm*, 1975 (*cryst struct*)
Wadsten, T., *Thermochim. Acta*, 1977, **21**, 285.

IC-000651

As_2SnZn
Tin zinc arsenide ($SnZnAs_2$), 9CI
Tin zinc diarsenide
[12006-34-7]

$ZnSnAs_2$

M 333.9
Exists as two forms; undergoes $\alpha \rightarrow \beta$ at 680-700°. Synth. from the elements heated in evacuated quartz ampoules. Semiconductor. Mp 775°.

α-form
Isostructural with chalcopyrite.

β-form
Zinc blende struct.

Vaipolin, A.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 974; *Inorg. Materials (Engl. Transl.)*, 1967, **3**, 871 (*synth*)
Veits, B.N. *et al*, *Latv. PSR Zinat. Akad. Vestis, Fiz. Teh Zinat. Ser.*, 1969, **2**, 60 (*mössbauer*)
Krivaite, G. *et al*, *Fiz. Tekh. Poluprov.*, 1971, **5**, 2242 (*reflectance*)
Khrostantsev, L.G. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1972, **206**, 1342 (*dec*)
Dittrich, V. *et al*, *Neue Haelbe*, 1972, **17**, 526 (*phase system*)
Kapralik, I., *Chem. Zvesti*, 1973, 2745 (*α, β-forms*)
Monfort, Y. *et al*, *Phys. Status Solidi A*, 1975, **29**, 551 (*cryst struct*)
Isomura, S., *Trans. Natl. Res. Inst. Met. (Jpn.)*, 1975, **17**, 98 (*elect props, synth*)
Brudnyi, V.N. *et al*, *Phys. Status Solidi A*, 1976, **35**, 425 (*semiconducting props*)
Mokronsov, G.M. *et al*, *Vapr. Khim. (Tausk)*, 1977, **12**, 60 (*synth*)

As_2Sn_3 IC-000652
Tin arsenide (Sn_3As_2)
[12255-99-1]

Sn_3As_2

M 505.9

Boltaks, B.I. *et al*, *Teor. Eksp. Khim.*, 1970, **6**, 424 (*mössbauer*)
Shipatov, V.T. *et al*, *Teor. Eksp. Khim.*, 1972, **8**, 413 (*mössbauer*)
Baidakov, L.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1977, **13**, 616; *CA*, **87**, 32874s (*magnetism*)
Szesny, B. *et al*, *Metall (Berlin)*, 1986, **40**, 868; *CA*, **105**, 212301k.

As_2Te_3 IC-000653
Arsenic telluride (As_2Te_3), 9CI, 8CI
Diarsenic(III) tritelluride. Tellurium arsenide. Arsenic sesquitelluride
[12044-54-1]

As_2Te_3

M 532.6
Monoclinic. Parallel layer struct. As(1) coordinated by 6 Te in distorted octahedron, As(2) by 7 Te as tetragonal prism and triangular prism with cojoint base. Also exists in amorphous and vitreous states. A new metastable, rhombohedral form has also been descr. Synth from As + Te. Semiconductor. Component of many laminar glasses. Promising material for memory devices. Commercially available. Grey, needle-like cryst. Mp 360°, Mp 381°.

Amorphous-form
Struct. approximates to that of cryst. form. Corrugated layers but no long-range order. Each As coordinated to 3 Te's, and each Te to 2 As's.

Vitreous-form
By drastic supercooling of melt. Mp 405-410°. Softening temp. *ca.* 140°.

Eifert, J.R. *et al*, *J. Mater. Sci.*, 1968, **3**, 293 (*phase diagram*)
Kravchenko, E.A. *et al*, *Phys. Status Solidi*, 1969, **31**, K19 (*nqr*)
Ban, V.S. *et al*, *J. Chem. Phys.*, 1970, **52**, 248 (*ms*)
Nabitovich, I.D. *et al*, *Kristallografiya*, 1976, **21**, 620; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1976, **21**, 348 (*cryst struct*)
Seregin, P.P. *et al*, *Fiz. Khim. Steckla*, 1977, **3**, 512; *Sov. J. Glass Phys. Chem. (Engl. Transl.)*, 1977, **3**, 470 (*pe*)
Uemura, O. *et al*, *J. Non-Cryst. Solids*, 1979, **33**, 71 (*nd*)
Kanishcheva, A.S. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1982, **18**, 949; *Inorg. Materials (Engl. Transl.)*, 1982, **18**, 796 (*cryst struct*)
Gosh, B. *et al*, *Prog. Cryst. Growth Charact.*, 1983, **6**, 393 (*cryst, props, rev*)
Stergiou, A.C. *et al*, *Z. Kristallogr.*, 1985, **172**, 139 (*synth, cryst struct*)
Shu, H.W. *et al*, *Mater. Res. Bull.*, 1986, **21**, 1509 (*cryst struct*)
Shu, H.W. *et al*, *J. Solid State Chem.*, 1988, **74**, 277.

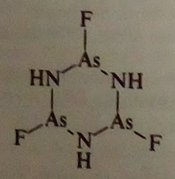
$As_3ClO_{12}Pb_5$ IC-000654
Lead arsenate chloride ($Pb_5(AsO_4)_3Cl$)
Mimetite

$Pb_5(AsO_4)_3Cl$

M 1488.2
Mineral: found as ore in New Jersey, Sweden, Czechoslovakia, Siberia, Italy and Germany. Cryst. Possesses hexagonal symmetry.

Foertsch, E., *Neues Jahrb. Mineral., Abh.*, 1970, **113**, 219 (*cryst struct*)
Brenner, P. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1970, **131**, 206 (*synth, cryst struct*)
Weitz, g., *Neues Jahrb. Mineral., Monatsh.*, 1971, 223.
Manca, S.G. *et al*, *Monatsh. Chem.*, 1980, **111**, 949 (*ir*)

$As_3F_3H_3N_3$ IC-000655
2,4,6-Trifluorohexahydro-*s*-triazatriarsinine, 8CI



M 326.8
Derivs. obt. from AsF_3 + RNH_2.

1,3,5-Triethyl: 1,3,5-Triethyl-2,4,6-trifluorohexahydro-1,3,5,2,4,6-triazatriarsinine
$C_6H_{15}As_3F_3N_3$ M 410.9
Colourless liq. Bp_{12} 180-182°. n_D^{20} 1.5752.

1,3,5-Triisopropyl: 2,4,6-Trifluorohexahydro-1,3,5-triisopropyl-1,3,5,2,4,6-triazatriarsinine
$C_9H_{21}As_3F_3N_3$ M 453.0
Colourless liq. Bp_9 150-159°. n_D^{20} 1.5492.

1,3,5-Tri-tert-butyl: 1,3,5-Tri-tert-butyl-2,4,6-trifluorohexahydro-1,3,5,2,4,6-triazatriarsinine
$C_{12}H_{27}As_3F_3N_3$ M 495.1
Colourless cryst. Mp 90-91°. Bp_8 91-92°.

Olah, G.A. *et al*, *Can. J. Chem.*, 1961, **38**, 1431.

IC-000656

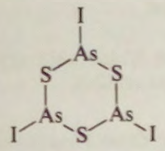
$As_3H_5O_{10}$
Triarsenic acid, 9CI, 8CI
Arsenic pentoxide hydrate (3:5)
[22538-92-7]

$H_5As_3O_{10}$

M 389.7
Triclinic. Possesses chain struct. formed from the AsO_4 tetrahedra (with As—O 167.6 pm) and AsO_6 octahedra (As—O 181.8 pm) by corner sharing. Formed from H_3AsO_4 aq. Colourless cryst., dehydrating at 170°.

Jost, K.-H. *et al*, *Acta Crystallogr.*, 1966, **21**, 808 (*synth, cryst struct*)

$As_3I_3S_3$ IC-000657
2,4,6-Triiodo-1,3,5,2,4,6-trithiatriarsenane, 9CI
Arsenic sulfoiodide cyclotrimer. Triarsenic triiodide trisulfide. Arsenic iodide sulfide ($As_3I_3S_3$)
[39399-59-2]



M 701.6
Detected in vapour above Arsenic iodide sulfide (AsIS), IC-000512.

Bakhyshev, R.G. *et al*, *Azerb. Khim. Zh.*, 1972, 137; *CA*, **79**, 10407.

$As_3K_5O_{10}$ IC-000658
Pentapotassium triarsenate, 10CI
Pentapotassium arsenate ($As_3O_{10}^{5\ominus}$), 9CI, 8CI
[60218-21-5]

$K_5(As_3O_{10})$

M 580.2
Orthorhombic. Groups of three corner-sharing AsO_4 tetrahedra form strongly bent chains. Coordination number of K is 6-9. From KH_2AsO_4 by heating at 600°, or from K_2O—As_2O_5 melt. Colourless, v. hygroscopic solid. Mp 680° (630°) (incongr.).

Gmelin Handbook Inorg. Chem., Syst. No. 22, 1936-8, 1026 (*rev, bibl*)
Verweij, H., *Appl. Spectrosc.*, 1979, **33**, 509 (*synth, ir, raman*)
Kasenov, B.K. *et al*, *Zh. Fiz. Khim.*, 1979, **53**, 2173; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1979, **53**, 1242.
Hornstra, J. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1634 (*synth, cryst struct*)

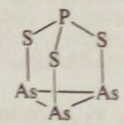
$As_3Na_5O_{10}$ IC-000659
Pentasodium triarsenate, 10CI
Pentasodium arsenate ($As_3O_{10}^{5\ominus}$), 9CI
[16835-80-6]

$Na_5(As_3O_{10})$

M 499.7
Polymorphic. From $NaAsO_3$ – Na_3AsO_4 system; Na_3AsO_4 + As_2O_5 at *ca.* 590-700°; $NaAsO_3$ + $Na_4As_2O_7$. Mp 680° (incongr.). $\alpha \rightarrow \beta \rightarrow \gamma$ polymorphic transitions at *ca.* 410° and 470-480°.

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1928, 948 (*rev, bibl*)
Beilina, A.Z. *et al*, *Zh. Fiz. Khim.*, 1976, **50**, 253; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 148 (*ir, raman*)
Isabaev, S.M. *et al*, *Zh. Neorg. Khim.*, 1976, **21**, 3134; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1728 (*synth, ir, raman, props*)
Kasenov, B.K. *et al*, *Zh. Fiz. Khim.*, 1985, **59**, 1528; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1985, **59**, 901 (*struct*)

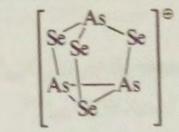
As_3PS_3 IC-000660
Arsenic phosphorus sulfide (As_3PS_3), 11CI
Triarsenic phosphorus trisulfide



M 351.9
Probable struct. shown. Synth. from P_4S_3 + As_4S_3 at 250° in sealed tube. Yellow cryst. Bp 190°.

Brockner, W. *et al*, *Z. Naturforsch., A*, 1981, **36**, 846 (*struct*)
Blachnik, R. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1493; 1984, **39**, 1135 (*synth, ms, P-31 nmr*)
Brunvoll, J. *et al*, *Z. Naturforsch., A*, 1982, **37**, 342 (*struct*)
Blachnik, R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 317 (*synth*)
Gimare, B. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 506 (*struct*)
Bues, W. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **516**, 42 (*synth, P-31 nmr*)
Operti, L. *et al*, *Inorg. Chim. Acta*, 1985, **96**, 43 (*ms*)
Baldus, H.P. *et al*, *Phosphorus Sulfur*, 1987, **30**, 361 (*synth*)

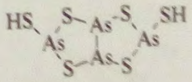
$As_3Se_4^{\oplus}$ IC-000661
[μ_3-Diseleno-*Se:Se:Se'*]di-μ-selenoxotriarsenic(1+), 10CI



M 540.6 (ion)
Hexafluoroarsenate: [77825-65-1].
$As_4F_6Se_4$ M 729.5
Synth. from As + Se melt, + AsF_5. Orange cryst. Not v. stable, and quickly darkens.
Hexafluoroantimonate: [77825-66-2].
$As_3F_6SbSe_4$ M 776.3
Synth. from As + Se melt, + SbF_5. Monoclinic. Orange, diamond-shaped plates. Interatomic distances: Se—Se 231.0, As—Se 232.0, 235.8, 246.4 pm.

Christian, B.H. *et al*, *Inorg. Chem.*, 1981, **20**, 3410 (*synth, ir, raman, cryst struct*)

$As_4H_2S_6$ IC-000662
Thioarsenic acid ($H_2As_4S_6$), 9CI
Thioarsenious acid, 8CI. Dihydrogen hexathiotetraarsenate. 2,6-Dimercapto[1,3,2,4,5]dithiatriarsolo[4,5-d][1,3,2,4,5]dithiatriarsole



M 494.0
Dipiperidinium salt: [25114-24-3].
$C_{10}H_{24}As_4N_2S_6$ M 664.3

From As_4S_4 (Arsenic sulfide (As_4S_4), IC-000668) and piperidine. Air-stable yellow cryst. Orthorhombic; interatomic distances: As—As 258, As—S (exocyclic) 218, As—S (endocyclic) 223, 230 pm.

Lauer, W. *et al, Z. Anorg. Allg. Chem.*, 1969, **371**, 193 (*synth*)
Porter, E.J. *et al, J. Chem. Soc. A*, 1971, 3130 (*cryst struct*)

IC-000663

$As_4I_2Te_8$

Arsenic iodide telluride ($As_4I_2Te_8$), 9CI, 8CI

[12349-94-9]

$As_4I_2Te_8$

M 1191.4
Synth. from As + I + Te at 600-900°. Exists as brown, needle-like cryst. or glass.

Vitreous-form
Polymeric chain struct. Mp 290-300°. Softens at 110-120°. Cryst. temp. 170°.

Demborskii, S.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1229; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1079 (*synth*)
Chernov, A.P. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 383 (*synth*)
Mel'nichenko, T.N. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 1065; *Inorg. Materials (Engl. Transl.)*, 1971, **7**, 945 (*synth, props*)
Vasil'ev, L.N. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1976, **12**, 350; *Inorg. Materials (Engl. Transl.)*, 1976, **12**, 302 (*synth, mössbauer*)
Seregin, P.P. *et al, Fiz. Khim. Steekla*, 1977, **3**, 512 (*pe*)
Archakev, Yu.I. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 1007; *Inorg. Materials (Engl. Transl.)*, 1978, **14**, 790 (*mössbauer, uv-vis*)
Kniep, R. *et al, Z. Naturforsch., B*, 1982, **37**, 151 (*phase diagram*)

IC-000664

$As_4KO_{140}W_{40}^{27\ominus}$

Tungstopotassioarsenate ($KAs_4W_{40}O_{140}^{27\ominus}$)

$[As_4KW_{40}O_{140}]^{27\ominus}$

M 9932.7 (ion)
A cryptate-type complex which encapsulates the K ion. Forms complexes with cytochrome C.

Heptacosa-Na salt: [68009-98-3]
$As_4KNa_{27}O_{140}W_{40}$ M 10553.4
Cryst.

Heptacosa-K salt: [68009-97-2].
$As_4K_{28}O_{140}W_{40}$ M 10988.3
Cryst.

Leyne, M. *et al, Nouv. J. Chim.*, 1978, **2**, 233 (*synth, uv, ir, raman*)
Chottard, G. *et al, Biochim. Biophys. Acta*, 1987, **916**, 402 (*binding, cytochrome C*)

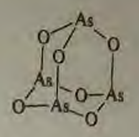
IC-000665

As_4O_6

Arsenic oxide (As_4O_6)

2,4,6,8,9,10-Hexaoxa-1,3,5,7-tetraarsaadamantane. 2,4,6,8,9,10-Hexaoxa-1,3,5,7-tetraarsatricyclo[3.3.1.1^{3,7}]decane, 9CI. Hexa-μ-oxotetraarsenic, 9CI. White arsenic. Arsenic trioxide (incorr.)

[12505-67-8]



M 395.6
Struct. exists in vap. phase. Interatomic distances: As—O 178.7; angles: OAsO 98.3°, AsOAs 128.0°. Isostructural with Phosphorus oxide (P_4O_6), IC-021484. Synth. from $AsCl_3$ + boiling H_2O. White cubic cryst. Mp 278°. Bp 465°. Condensation of vap. at >250° gives vitreous As_2O_3. Cubic struct. retained if rapid condensation at <250°. At > 800° vap. partly → Arsenic oxide (As_2O_3), IC-000627 and dissoc. increases with temp. When heated at 180° with trace H_2O, is converted into Arsenic oxide (As_2O_3), IC-000627. ΔH_f° −657 kJ mol^{-1}.

Monoxide: [86508-52-3].
As_4O_5 M 411.6
Det. in As_2O_3 vap. at 600-700°. Isol. in matrix.

1,3-Dioxide: [106611-12-5].
As_4O_8 M 427.6
Isol. in matrix.

1,3,5-Trioxide: [86508-53-4].
As_4O_9 M 443.6
Det. in As_2O_3 vap. at 600-700°. Isol. in matrix.

Tetraoxide: [12355-85-0]. *Arsenic pentoxide (incorr.). Tetraoxohexa-μ-oxotetraarsenic*
As_4O_{10} M 459.6
Det. in As_2O_3 vap. at 600-700°. Isol. in matrix.

Mineral-form [1303-24-8]
Arsenolite
Secondary mineral. Cubic white cryst., also tinted yellowish, bluish or reddish.

[36533-93-4]

Brumbach, S.B. *et al, J. Chem. Phys.*, 1972, **56**, 3110 (*raman*)
Diemann, E., *Inorg. Chim. Acta*, 1977, **24**, L27 (*pe*)
Pertlik, F., *Czech. J. Phys.*, 1978, **B28**, 170; *CA*, **88**, 113743 (*cryst struct*)
Rytter, E. *et al, J. Chem. Phys.*, 1978, **69**, 3717 (*raman*)
Sourisseau, C. *et al, Spectrochim. Acta, Part A*, 1978, **34**, 173 (*raman*)
Egdell, R.G. *et al, Inorg. Chem.*, 1980, **19**, 1314 (*pe*)
Bradaczek, H. *et al, Ber. Bunsenges. Phys. Chem.*, 1981, **85**, 369 (*props*)
Plies, V. *et al, Z. Anorg. Allg. Chem.*, 1983, **497**, 185 (*ms, oxides*)
Brisdon, A.K. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 2725 (*oxides*)
Rose, J.L. *et al, J. Phys. Chem.*, 1989, **93**, 3504 (*uv*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 305.

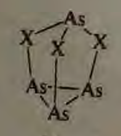
IC-000666

As_4S_3

Arsenic sulfide (As_4S_3), 9CI, 8CI

Tetraarsenic(III) trisulfide. 3,5,7-Trithia-1,2,4,6-tetraarsatricyclo[2.2.1.0^{2,6}]heptane

[12512-13-9]



X = S

M 395.8
Dimorphic. Mean interatomic distances: As—As 245, As—S 221 pm. Yellow to orange solid. At <130°, β form → α form.

Mineral-form [1303-41-9]
Dimorphite
Known in two modifications. α-Dimorphite (Dimorphite I) is identical to synthetic As_4S_3. Dimorphite II (β-As_4S_3) is orthorhombic with As—As 247.0 pm. Yellow-orange solid.

Whitfield, H.J., *J. Chem. Soc. A*, 1970, 1800 (*cryst struct*)
Whitfield, H.J., *Aust. J. Chem.*, 1971, **24**, 697 (*ir*)
Bastow, T.J. *et al, Aust. J. Chem.*, 1972, **25**, 2291 (*nqr*)

Whitfield, H.J., *J. Chem. Soc., Dalton Trans.*, 1973, 1737 (*cryst struct*)
Frankel, L.S. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1973, **138**, 161 (*cryst struct*)
Blachnik, R. *et al, Z. Anorg. Allg. Chem.*, 1980, **463**, 78 (*phase diagram*)
Bues, W. *et al, Z. Naturforsch., B*, 1980, **35**, 1063 (*ir, raman*)
Christian, B.H. *et al, Inorg. Chem.*, 1981, **20**, 3410 (*raman*)

IC-000667

As_4S_4

Arsenic sulfide (As_4S_4)

2,4,7,8-Tetrathia-1,3,5,6-tetraarsatricyclo[3.2.1.0^{3,6}]octane. γ-Tetraarsenic tetrasulfide

M 427.9
Interatomic distances (mean): As—As 253.5, As—S 224.4 pm; angles: AsSAs 105.2°, SAsS 101.2°, AsAsS 95.8°, AsAsAs 83.2°. From As + S at 500-600° with subsequent rapid cooling. Yellow orange plates (CS_2). Mp 318° (307°).

Kutoglu, A., *Z. Anorg. Allg. Chem.*, 1976, **419**, 176 (*synth, cryst struct*)

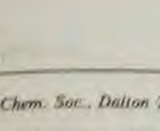
IC-000668

As_4S_4

Arsenic sulfide (As_4S_4), 9CI, 8CI

2,4,6,8-Tetrathia-1,3,5,7-tetraarsatricyclo[3.3.0.0^{3,7}]octane

[12279-90-2]



M 427.9
Arsenic atoms arranged tetrahedrally with the sulfide atoms almost coplanar. Mean interatomic distances, As—S 259.3, As—S 224.3 pm. In vap., mean As—As 249 pm.

α-form [12044-30-3]
Realgar
Mineral. Found as pigment in ancient Persian and Armenian manuscripts. Widespread occurrence, e.g. in Sb ores of Yugoslavia; hot spring deposits in USSR; borate deposits in Turkey; gold ores of USA (Montana) and Armenia. Orange-red solid. At 270°, → β-form. On exp. to light, → orpiment.

β-form
Synthetic-form
Molecular packing not identical to that of α-form. Synth. from As + S at 400-1000° under pressure. Cryst. (CS_2 or C_6H_6). Mp 320°. Bp 565°. Subl. *in vacuo*. Annealing at 200° → α-form. In vap., dissociation into As_2S_2 complete at 1000°. Colour of solid darkens at >170°.

Lu, C.-S. *et al, J. Am. Chem. Soc.*, 1944, **66**, 818 (*ed*)
Forneris, R., *Am. Mineral.*, 1969, **54**, 1062 (*ir, raman*)
Munir, Z.A. *et al, J. Chem. Phys.*, 1971, **55**, 4520 (*ms*)
Yu, S. *et al, Am. Mineral.*, 1972, **57**, 1873 (*cryst struct*)
Stec, W.J. *et al, Inorg. Chem.*, 1972, **11**, 219 (*pe*)
Porter, E.J. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1347 (*cryst struct*)
Bastow, T.J. *et al, Solid State Commun.*, 1977, **11**, 1015 (*nqr, tr*)
Mullen, D.J.E. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1972, **136**, 48; 1974, **140**, 27 (*cryst struct, rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 582 (*synth*)
Christian, B.H. *et al, Inorg. Chem.*, 1981, **20**, 3410 (*raman, reactions*)

IC-000669

As_4S_5

Arsenic sulfide (As_4S_5), 9CI, 8CI

Tetraarsenic pentasulfide. 2,6-Epithio[1,3,2,4,5]dithiatriarsolo[4,5-d][1,3,2,4,5]dithiatriarsole. 1,3,5,7-Tetraarsa-2,4,6,8-tetrathiatricyclo[3.3.1.0^{3,7}]nonane

[25114-28-7]

M 460.0
Interatomic distances: As—As 255, As—S 224 pm. Synth. from As_4S_3 + S in CS_2. Orange needle-like monoclinic cryst.

Lauer, W. *et al, Z. Anorg. Allg. Chem.*, 1969, **371**, 193 (*form*)
Whitfield, H.J., *J. Chem. Soc., Dalton Trans.*, 1973, 1740 (*synth, cryst struct*)
Yanabe, T. *et al, Solid State Commun.*, 1981, **40**, 521 (*struct*)

IC-000670

As_4Se_3

Arsenic selenide (As_4Se_3), 10CI

Tetraarsenic(III) triselenide. 3,5,7-Triselena-1,2,4,6-tetraarsatricyclo[2.2.1.0^{2,6}]heptane

[63897-50-7]

As Arsenic sulfide (As_4S_3), IC-000666 with

X = Se

M 536.5
From As + Se at 220°.

α-form
Dark-red orthorhombic cryst. isostructural with α-Arsenic sulfide (As_4S_3), IC-000666.

β-form
Red monoclinic cryst.

Bastow, T.J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 959 (*synth, cryst struct, nqr*)
Blachnik, R. *et al, Z. Anorg. Allg. Chem.*, 1980, **463**, 78 (*phase diagram*)
Blachnik, R. *et al, Thermochim. Acta*, 1984, **81**, 185 (*props*)
Operti, L. *et al, Inorg. Chim. Acta*, 1985, **96**, 43 (*ms*)

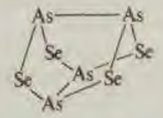
IC-000671

As_4Se_4

Arsenic selenide (As_4Se_4), 9CI, 8CI

Tetraarsenic tetraselenide

[52126-83-7]



M 615.5

Isomorphous with Realgar. Monoclinic, interatomic distances: As—As 256.5, As—Se 238.8 pm. Synth. from As + Se at 500°, annealed at 250°. Black, rod-like cryst. (by sublm.). Dec. at 264° to Arsenic selenide (As_2Se_3). IC-000649 together with a lig.

[12279-91-3]

Myers, M.B. *et al, Mater. Res. Bull.*, 1967, **2**, 715 (*phase diagram*)
Kravchenko, E.A. *et al, Phys. Status Solidi*, 1969, **31**, K19 (*sapr*)
Renninger, A.L. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 1583 (*cryst struct*)
Smith, E.J. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 2014 (*synth, cryst struct*)
Barrow, T.J. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1739 (*synth, cryst struct*)
Goldstein, P. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 915 (*synth, cryst struct*)
Salanek, W.R. *et al, Phys. Rev. B*, 1975, **12**, 725.
Buss, W. *et al, Z. Anorg. Allg. Chem.*, 1983, **499**, 7 (*raman*)

As_2ITe_2 IC-000672

Arsenic iodide telluride (As_2ITe_2), 11Cl

[81858-63-1]

As_2ITe_2

M 1394.7

Contains chains of condensed polyhedra. Three As atoms are octahedrally coordinated by six Te or I atoms. The other two As atoms enclosed by polyhedra of 7 Te atoms consisting of tetragonal pyramid and triangular prism sharing common face. Synth. from As + Te + HI (aq.) at 320° in sealed tube, or from As_2Te_3 + AsI_3 at 300–400°. Grey, needle-like cryst.

Krebs, B. *et al, Z. Naturforsch., B*, 1982, **37**, 151 (*synth, cryst struct*)
Bärnighausen, A.C. *et al, Z. Kristallogr.*, 1985, **172**, 111 (*synth, struct*)

$As_2Pb_2S_5Tl$ IC-000673

Rathite

[12174-39-9]

$(Pb,Tl)_2As(As,Ag)S_5$

M 1314.0

Mineral found in Swiss ores (Binnes Valley deposit). Lead-grey metallic cryst.

Kraus, A., *Bull. Soc. Frib. Sci. Nat.*, 1974, **63**, 139
Ozawa, T. *et al, Neues Jahrb. Mineral., Monatsh.*, 1974, 530 (*cryst struct*)
Friedrich, M., *Bel. Geowiss. Abh., Reihe A*, 1983, **46**, 109.

$As_2O_{28}V_4^{10-}$ IC-000674

Tetrakis(μ-[orthoarsenato(3−)-*O*:*O'*]]bis[μ-[orthoarsenato(3−)-*O*:*O*:*O'*:*O'*]]di-μ-oxotetravanadate(*III*)(10−), 11Cl

$[V_4O_2(AsO_4)_4]^{10-}$

M 1069.2 (ion)

Struct. includes two pairs of edge-shared VO_5 octahedra joined by tetrahedral AsO_4 units.

Tetra-NH₄ salt, hexa-H compd., tetrahydrate: [70956-73-9]. Synth. by dissolving V_2O_5 in aq. arsenic acid then adding $(NH_4)_2CO_3$. Orange solid.

Durif, A. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 1441 (*synth, cryst struct*)
Lavrov, A.E. *et al, Acta Stat. Am. Quim.*, 1981, **1**, 77; *CA*, **96**, 225616m (*ir, raman*)

$As_4H_4N_2S_{13}$ IC-000675

Ammonium arsenic sulfide, 11Cl

$(NH_4)_2(As_2S_{13})$

M 1052.3

Monohydrate: [99399-32-3].

Synth. from As_2S_3 + $(NH_4)_2CO_3$ aq. in sealed tube at 220°. Monoclinic. Isotypic with corresp. Rb salt. Polymeric anion $(As_2S_{13}^{2\ominus})_n$ consists of individual As_2S_3 rings connected via bridging AsS_3 pyramids.

Sheldrick, W.S. *et al, Z. Naturforsch., B*, 1985, **40**, 1130 (*synth, struct*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 302.

$As_4Pb_9S_{18}$ IC-000676

Lead arsenide sulfide ($Pb_9As_4S_{18}$)

Baumhauerite

[1303-40-8]

$Pb_9As_4S_{18}$

M 2212.5

Arsenic is coord. by S in trigonal pyramid. 12 Independent Pb atoms: 8 have 9S atoms, 4 have 7S atoms. AsS_3 pyramids form finite chains. Mineral found in Binna Valley deposit, Switzerland. Cryst.

Nakai, I. *et al, Proc. Int. Symp. Hydrotherm. React. (1st, 1982)*, 772 (*synth*)
Jambor, J.L., *Can. Mineral.*, 1968, **9**, 505 (*synth*)
Engel, P. *et al, Z. Kristallogr.*, 1969, **129**, 178 (*cryst struct*)
Walia, D.S. *et al, Can. Mineral.*, 1973, **12**, 113.
Maijs, L., *Latv. PSR Zinat. Akad. Vestis, Khim. Ser.*, 1979, 162.
Friedrich, M., *Bel. Geowiss. Abh., Reihe A*, 1983, **46**, 109.

At IC-000677

Astatine

Diastatine

[7440-68-8]

At_2

M 209.9

Atomic No. 85. Ground state electron config. [Xe] $4f^{14}5d^{10}6s^26p^5$. Obt. by D.R. Carson, *et al* (1940). Rarest naturally occurring terrestrial element. At least 20 radioactive isotopes known. Longest half life ^{210}At 8.3 hrs. Obt. by bombarding ^{209}Bi with energetic alpha particles. Only microgram quantities have been prepd. Oxidation states −1, 0, +1, +3, +5 known. Sol. H_2O, C_6H_6, CCl_4. Mp 302°. Bp 337° (230°).

Mellor Compr. Treat. Inorg. Theor. Chem., Suppl. 1, 1956, 1064 (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1107 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **19**, 652 (*rev, bibl*)
Greenwood, N.N. *et al, Chemistry of the Elements*, 1986, 920 (*rev*)
Visser, G.W.M., *Radiochim. Acta*, 1989, **47**, 97 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 24.

Au IC-000678

Gold

Aurum (L.)

[7440-57-5]

Au

M 196.9

Atomic No. 79. Ground state electron config. [Xe]

$4f^{14}5d^{10}6s^1$. 27 Isotopes are known of which only one, ^{197}Au, is stable. Known to ancient civilisations. Has no biological role. The most electronegative metal. Abundance: 0.004 ppm (earth's crust), 4×10^{-4} ppm (sea water). Has fcc struct. Occurs as native Au or as tellurides. Extracted with Hg or by the cyanide process and pptd. with Zn. Excellent electrical and thermal conductor. Main uses in dentistry, jewellery, electronics and aerospace industries, and as bullion. Soft, yellow, malleable, ductile metal. Forms red, blue or violet colloidal suspensions. Physical props. depend on mechanical treatment. Mp 1064°. Bp 2808°. Stable in dry air at r.t.; and to H_2O, acids (except HNO_3/HCl) and alkalis. Sol. in aq. $CN^{\ominus}$. Unreactive to O_2, S, Se but reacts with Te.

P Non toxic. MD5070000

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1923, **3**, 491 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 62, 1954 (*rev, bibl*)
Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 3 (*history*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **3**, 129 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 971 (*synth, recovery*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **11**, 972 (*rev, bibl*)
Greenwood, N.N. *et al, Chemistry of the Elements*, Pergamon, Oxford, 1986, 1364 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 80.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1818.

|AuBa| IC-000679

Barium-gold system

Alloy with two main phases.

Barium gold [66983-46-8]

AuBa M 334.2

Orthorhombic; isostructural with FeB with zigzag chains of atoms.

Barium gold (Ba₃Au₂) [102678-03-5]

Tribarium digold. ***Barium compd. with gold (2:3), 11Cl***

Au_2Ba_3 M 805.9

Er_3Ni_2 struct. type.

Fornasini, M.L. *et al, J. Solid State Chem.*, 1985, **59**, 60 (*synth, cryst struct*)
Fornasini, M.L. *et al, Rev. Chim. Minér.*, 1986, **22**, 791 (*cryst struct*)

|AuBe| IC-000680

Beryllium-gold system

Alloy with two main phases.

Beryllium compd. with gold (1:3) [66104-14-1]

Beryllium trigold

Au_3Be M 599.9

Beryllium compd. with gold (1:1), 11Cl [12044-69-8]

Beryllium gold

AuBe M 205.9

Kao, S.G. *et al, K'uang Yeh*, 1981, **25**, 125; *CA*, 1982, **96**, 10323d (*synth, Au_3Be*)
Borisov, Yu.A., *Zh. Strukt. Khim.*, 1983, **24**, 97 (*theory*)
Chin, A.K. *et al, Appl. Phys. Lett.*, 1984, **45**, 37 (*contacts*)

AuBr IC-000681

Gold(*I*) bromide (AuBr), 10Cl

[10294-27-6]

AuBr

M 276.8

Struct. comprises zig-zag chain of linear gold(*I*) moieties. Cryst. obtained by vapour transport techniques with Br_2 pressures of 2 atm. (210-240°). Occurs in two tetragonal cryst. modifications.

Belton, P.A. *et al, Zh. Prikl. Spektrosk.*, 1977, **26**, 980 (*art*)
Janssen, E.M.W. *et al, J. Less-Common Met.*, 1978, **57**, 247, 255 (*cryst struct, phase trans*)

AuBrSe IC-000682

Gold(*III*) bromide selenide (AuBrSe), 9Cl

[34998-72-2]

AuBrSe

M 355.8

Ribbon struct. with square planar gold(*III*) atoms. Two independent gold sites, one coordinated to two Se and two Br and the other by four Se. Synth. by heating Au and Se in presence of Br_2 in 230-200° temperature gradient. Dark grey metallic cryst.

Rabenau, A. *et al, Monatsh. Chem.*, 1971, **102**, 1425 (*synth*)
Moore, J. *et al, J. Solid State Chem.*, 1975, **4**, 383 (*cryst struct*)

$AuBrTe_2$ IC-000683

Gold bromide telluride ($AuBrTe_2$)

[12523-46-9]

$AuBrTe_2$

M 532.0

Silvery white cryst. with metallic conductivity.

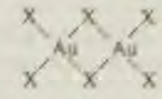
Rabenau, A. *et al, J. Less-Common Met.*, 1970, **21**, 395
Inorg. Synth., 1973, **14**, 160 (*synth*)
Haendler, H.M. *et al, J. Solid State Chem.*, 1974, **10**, 175
Zhou, B.L. *et al, J. Phys. C*, 1981, **14**, 4393 (*electronic props*)

$AuBr_3$ IC-000684

Gold(*III*) bromide ($AuBr_3$), 10Cl

Gold tribromide. Auric bromide

[10294-28-7]



dimer X = Br

M 436.6

Dimeric.

Dimer: [11092-53-8]. *Di-μ-bromotetrabromodigold, 9Cl*

Hexabromodigold

Au_2Br_6 M 873.3

Synth. from gold and excess Br_2 in sealed ampoule at 140° over 4 d. Commercialy available. Dark-red to black cryst. Hydrol. rapidly in moist air.

Batsanov, S.S. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1971, 1863 (*dimer*)
Lörcher, K.-P. *et al, Z. Naturforsch., B*, 1975, **30**, 662 (*synth, cryst struct*)
Fokina, Z.A., *Koord. Khim.*, 1980, **6**, 1463 (*synth*)

$AuBr_4^{\ominus}$ IC-000685

Tetrabromoaurate(*III*)(1−), 9Cl

[14337-14-5]

$[AuBr_4]^{\ominus}$

M 516.5 (ion)

K salt: [14323-32-1]. *Potassium bromoaurate*
$AuBr_4K$ M 555.6
Prepd. from KBr + Au + Br_2. Commercially available. Reddish-purple cryst. Slowly absorbs water from the atm. to give the dihydrate. V. sol. H_2O, MeOH, EtOH. Mp 120° dec.

H compd: [17083-68-0]. *Bromoauric acid*
$AuBr_4H$ M 517.5
Formed from $AuBr_3$ + aq. HBr. Very hygroscopic, dark red cryst. (+$5H_2O$). V. sol. H_2O; sol. EtOH. Mp 80° dec.

[13005-38-4]

Inorg. Synth., 1953, **4**, 14 (*synth, K salt*)
Sabatini, A. *et al, Inorg. Chem.*, 1964, **3**, 1775 (*ir*)
Ito, H. *et al, Bull. Chem. Soc. Jpn.*, 1967, **40**, 2584 (*uv*)
Faltens, M.O. *et al, J. Chem. Phys.*, 1970, **53**, 4249 (*mössbauer*)
Bosworth, Y.M. *et al, Inorg. Chem.*, 1975, **14**, 170 (*raman*)
Straehle, J. *et al, Z. Anorg. Allg. Chem.*, 1979, **456**, 241 (*cryst struct, K salt*)
Cattalini, L. *et al, Inorg. Chem.*, 1985, **24**, 3409 (*synth, H compd*)
Omrani, H. *et al, Acta Crystallogr., Sect. C*, 1986, **42**, 1091 (*cryst struct, K salt, dihydrate*)

[AuCa] IC-000686

Calcium-gold system

Alloy with varying stoichiometry.

Calcium compd. with gold (1:5) [12006-70-1]
Au_5Ca M 1024.9

Calcium compd. with gold (2:9) [97397-31-4]
Au_9Ca_2 M 1852.8

Calcium compd. with gold (2:7) [97397-30-3]
Au_7Ca_2 M 1458.9

Calcium compd. with gold (1:3) [82678-78-2]
Au_3Ca M 630.9

Calcium compd. with gold (1:2) [12523-45-4]
Au_2Ca M 434.0

Calcium compd. with gold (1:1), 11CI [62683-54-9]
AuCa M 237.0
Isostructural with CrB.

Calcium compd. with gold (5:4) [98240-00-7]
Au_4Ca_5 M 988.2
Monoclinic with struct. based on $AuCa_6$ trigonal prisms linked in pairs through triangular faces. $CaCa_8$ cubes also present.

Calcium compd. with gold (5:3) [93509-35-4]
Au_3Ca_5 M 791.2
Tetragonal Cr_5B_3 struct. type.

Calcium compd. with gold (7:3) [98239-99-7]
Au_3Ca_7 M 871.4
Orthorhombic with struct. based on $AuCa_6$ trigonal prisms. Each gold has 9 Ca neighbours (tricapped trigonal prism arrangement).

Calcium compd. with gold (5:2) [102678-01-3]
Au_2Ca_5 M 594.3
Monoclinic Mn_5C_2 struct. type.

Calcium compd. with gold (3:1) [102678-00-2]
$AuCa_3$ M 317.2
Fe_3Ca struct. type.

Merlo, F. *et al, J. Less-Common Met.*, 1982, **86**, 241 (*cryst struct*)
Borisov, Yu.A. *et al, Zh. Strukt. Khim.*, 1983, **24**, 97 (*theory*)
Merlo, F. *et al, Rev. Chim. Minér.*, 1984, **21**, 273 (*cryst struct*)
Egan, J.J. *et al, High Temp. Sci.*, 1985, **19**, 111 (*thermodynamics of mixing*)
Fornasini, M.L. *et al, J. Solid State Chem.*, 1985, **59**, 65 (*cryst struct*)
Fornasini, M.L. *et al, Rev. Chim. Minér.*, 1986, **22**, 791 (*cryst struct, rev*)

[AuCd] IC-000687

Cadmium-gold system

Alloy with three main phases.

Cadmium compd. with gold (1:3) [12006-68-7]
Au_3Cd M 703.3
α_1-phase face centred tetragonal; α_2-phase hcp Mg struct.

Cadmium compd. with gold (1:1) [12044-73-4]
Gold cadmium
AuCd M 309.3
β-(high temp.) phase ordered b.c.c. CsCl struct., β'-phase is orthorhombic.

Cadmium compd. with gold (3:1) [62228-72-2]
$AuCd_3$ M 534.2

Metals Handbook, 8th Ed., 1973, **8**, 266 (*phase diagram*)
Hirabayashi, M. *et al, Electron Microsc. Proc. Eur. Congr. 7th*, 1980, **4**, 142; *CA*, 1982, **96**, 10382x (*electron microsc*)
Simic, V. *et al, J. Less-Common Met.*, 1983, **95**, 259 (*formn at bulk metal interface*)
Chulkov, E.V. *et al, Fiz. Met. Metalloved.*, 1985, **59**, 730; *CA*, 102, 224448q (*theory*)

AuCl IC-000688

Gold(*I*) chloride (AuCl), 10CI

[10294-29-8]

AuCl

M 232.4
Structure comprises zig-zag chain of linear gold moieties. Large cryst. obt. by vapour transport. Metastable with respect to disproportionation at r.t. to Au and Au_2Cl_6.

Janssen, E.M.W. *et al, J. Less-Common Met.*, 1974, **38**, 71 (*synth, cryst struct*)
Strähle, J. *et al, Z. Naturforsch., B*, 1974, **29**, 266 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1012 (*synth*)
Komiya, S. *et al, J. Organomet. Chem.*, 1977, **135**, 65 (*reactions*)

AuClO IC-000689

Gold chloride oxide (AuClO), 10CI

Gold(III) *oxide chloride*

[54220-51-8]

AuClO

M 248.4
Polymer consisting of linked hexameric rings, of alternating Au and O atoms. Au atoms are square-planar and bonded to one Cl and 3 O atoms. Obt. from Au_2O_3 with conc. $HClO_4$ at 160° in sealed pyrex tube. Red prismatic cryst. Mp 290° dec.

Schwarzmann, E. *et al, Z. Naturforsch., B*, 1974, **29**, 561 (*synth, ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1016 (*synth*)
Jones, P.G. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 2380 (*cryst struct*)
Jones, P.G. *et al, Gold Bull.*, 1980, **13**, 56 (*rev*)

$AuClO_3Se$ IC-000690

Gold chloride selenite, 11CI

Gold(III) *selenite chloride*

[83214-83-9]

$Au(SeO_3)Cl$

M 359.3
Has layer structure with AuO_3Cl, AuO_2Cl_2 and AuO_4 moieties. Synth. from $Au_2Se_4O_{11}$ at 280° in sealed tube. Air stable cryst.

Jones, P.G. *et al, Z. Naturforsch., B*, 1982, **371**, 941 (*synth, cryst struct*)

$AuClTe_2$ IC-000691

Gold chloride telluride ($AuClTe_2$), 9CI

Gold chloride ditelluride

[12523-42-1]

$AuTe_2Cl$

M 487.6
Formulated as $[Au(III)(Te_2)_{4/4}]Cl$. Each gold atom is coordinated to four Te_2 units and each Te_2 unit to four gold atoms, leading to a corrugated two dimensional net of Au and Te atoms. Silvery white cryst.

Rabenau, A. *et al, J. Less-Common Met.*, 1970, **21**, 395 (*synth*)
Inorg. Synth., 1973, **14**, 160 (*synth*)
Haendler, H.M. *et al, J. Solid State Chem.*, 1974, **10**, 175 (*cryst struct*)

$AuCl_3$ IC-000692

Gold(*III*) chloride ($AuCl_3$), 10CI

Gold trichloride. Auric chloride

[13453-07-1]

As Gold(*III*) bromide ($AuBr_3$), IC-000684 with

X = Cl

M 303.3
Dimeric in solid state and vapour phases. Intercalates into graphite.

▷MD5420000.

Dimer: [21563-00-8]. *Di-μ-chlorotetrachlorodigold, 10CI. Hexachlorodigold*
Au_2Cl_6 M 606.6
Synth. from the elements. Commercially available. V. hygroscopic orange-red cryst. (by subl.). Mp 200°.

Clark, E.S. *et al, Acta Crystallogr.*, 1958, **11**, 284 (*synth, cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1013 (*synth*)
Vangelesti, R. *et al, Carbon*, 1977, **15**, 327 (*intercalation compd*)

$AuCl_3H_3N$ IC-000693

Amminetrichlorogold(*III*)

Gold(III) *chloride ammine*

H_3NAuCl_3

M 320.3
Square planar struct. Interatomic distances: Au—N 201.2, Au—Cl 228.7, 228.2, 227.7 pm. Formed by thermal dec. of NH_4AuCl_4. Light yellow-green cryst. Dec. to metallic gold above 165°.

Strähle, J. *et al, Z. Anorg. Allg. Chem.*, 1979, **456**, 241 (*synth, cryst struct, ir*)

$AuCl_4^{\ominus}$ IC-000694

Tetrachloroaurate(*III*)(1 –), 9CI

[14337-12-3]

$[AuCl_4]^{\ominus}$

M 338.7 (ion)

Na salt: [15189-51-2]. *Sodium chloroaurate*
$AuCl_4Na$ M 361.7
Prepd. from $HAuCl_4$ + NaCl. Orange-yellow cryst. + $2H_2O$. V. sol. H_2O; sol. EtOH, Et_2O.
▷CK6360000.

K salt: [13682-61-6]. *Potassium chloroaurate*
$AuCl_4K$ M 377.8
Prepd. from $HAuCl_4$ + KCl. Commercially available. Air-stable, light-yellow cryst. + $2H_2O$. Sol. H_2O, EtOH; insol. Et_2O.

H compd: [16903-35-8]. *Chloroauric acid*
$AuCl_4H$ M 339.7
Formed when $AuCl_3$ is dissolved in HCl and when Au is dissolved in aqua regia. Used in photography and in gold plating baths. V. hygroscopic, deliquescent, light-yellow needles + $4H_2O$. V. sol. H_2O, EtOH; sol. Et_2O.

Hendra, P.J., *J. Chem. Soc. A*, 1967, 1298 (*ir, raman*)
Faltens, M.O. *et al, J. Chem. Phys.*, 1970, **53**, 4249 (*mössbauer*)
Bonamico, M. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 1735 (*cryst struct, K salt*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1014 (*synth, H compd*)
Theobald, F. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 2932 (*cryst struct, K salt, dihydrate*)
Jones, P.G. *et al, Acta Crystallogr., Sect. C*, 1988, **44**, 1164 (*cryst struct, Na salt*)

$AuCl_4P$ IC-000695

Chloro(phosphorous trichloride)gold, 9CI

Chloro(trichlorophosphine)gold(I). *Gold*(I) *chloride trichlorophosphine*

[60949-98-6]

Cl_3PAuCl

M 369.7
Struct. comprises zig-zag chains of linear Cl_3PAuCl molecules. V. moisture-sensitive white cryst. solid ($SOCl_2$).

Arai, G.J., *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1962, **81**, 307 (*cryst struct*)
Dell'Amico, D.B. *et al, Gazz. Chim. Ital.*, 1973, **103**, 1099 (*synth*)
Jones, P.G. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1430, 1439 (*mössbauer, synth, npr*)

AuCs IC-000696

Caesium gold (CsAu)

Gold compd. with caesium (1:1), 10CI

[12256-37-0]

CsAu

M 329.8
Has the CsCl struct. Sometimes regarded as $Cs^{\oplus}Au^{\ominus}$. Bright yellow alloy. Semi-conductor with excess Cs in lattice primary source of conduction electrons.

Tinelli, G.A. *et al, J. Solid State Chem.*, 1978, **25**, 157 (*cryst struct, Cs-133 nmr*)
Wertheim, G.K. *et al, Phys. Rev. B: Solid State*, 1979, **20**, 860 (*esca, mössbauer*)
Dupree, R. *et al, Phys. Rev. Lett.*, 1980, **45**, 130 (*Cs-133 nmr*)
Busse, B. *et al, Ber. Bunsenges. Phys. Chem.*, 1981, **85**, 309 (*gas phase dimer*)
Lowther, J.E., *Phys. Lett. A*, 1981, **81**, 470 (*theory*)

Batchelor, R.J. *et al*, *Hyperfine Interact.*, 1986, **28**, 955 (*mössbauer*)
Batchelor, R.J. *et al*, *Inorg. Chem.*, 1986, **25**, 2009 (*synth, mössbauer*)

IC-000697

AuCsO
Caesium gold(*I*) oxide, 11Cl
[23324-67-6]

CsAuO

M 345.8
Moisture-sensitive yellow solid. Tetragonal.
Wasel-Nielen, H.D. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **359**, 36 (*synth*)
Klassen, H. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **485**, 101 (*rev*)

IC-000698

AuF_3
Gold(*III*) fluoride (AuF_3), 9Cl
Gold trifluoride
[14720-21-9]

AuF_3

M 253.9
Helical fluorine bridged polymer, square planar about gold, but with weak cross linking between chains. Synth. from Au and F_2 in monel vessel at 350°. Golden yellow needles (by subl.).
Sharpe, A.G., *J. Chem. Soc.*, 1949, 2901 (*synth*)
Einstein, F.W.B. *et al*, *J. Chem. Soc. A*, 1967, 478 (*synth, cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 250 (*synth*)
Gabuda, S.P. *et al*, *Zh. Strukt. Khim.*, 1977, **18**, 515 (*F-19 nmr*)

IC-000699

$AuF_4^\ominus$
Tetrafluoroaurate(*III*)(1−)

$[AuF_4]^\ominus$

M 272.9 (ion)
Square planar Au(*III*).
Na salt: [31241-07-3].
AuF_4Na M 295.9
K salt: [24887-81-8].
AuF_4K M 312.0
Synth. from BrF_3, gold powder and KCl. Yellow cryst.
Edwards, A.J. *et al*, *J. Chem. Soc. A*, 1969, 1936 (*synth, cryst struct*)
Charlton, J.S. *et al*, *J. Chem. Soc. A*, 1970, 1484 (*mössbauer*)
Hoppe, R. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **379**, 122 (*cryst struct*)

$AuF_6^\ominus$ **IC-000700**
Hexafluoroaurate(1−)

$[AuF_6]^\ominus$

M 310.9 (ion)
Unusual example of octahedral Au(*V*).
Cs salt: [39043-78-2].
$AuCsF_6$ M 443.8
Can be obt. directly from $CsAuF_4$ and F_2.
$O_2^\oplus$ salt: [37237-60-8].
AuF_6O_2 M 342.9
Synth. from $CsAuF_4$, O_2 and F_2.
$Xe_2F_{11}^\oplus$ salt: [39043-77-1].
$AuF_{17}Xe_2$ M 782.5

Synth. from AuF_3, F_2 and XeF_6 at 400° and 70 atm. Pale yellow-green cryst. Mp 145-150°.
Leary, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1972, 903; 1973, 131 (*cryst struct, synth, ir, raman*)

IC-000701

[AuGa]
Gallium-gold system
Alloy with five main phases.
***Gallium compd. with gold* (*1:3*)** [83231-92-9]
Gallium trigold. Gallium gold (*$GaAu_3$*). *Gold gallium* (*Au_3Ga*)
Au_3Ga M 660.6
Gallium compd. with gold* (*1:2*), *11Cl [54327-67-2]
Gallium digold. Gallium gold (*$GaAu_2$*). *Digold gallium*
Au_2Ga M 463.6
Gallium compd. with gold* (*1:1*), *11Cl [12006-53-0]
AuGa M 266.6
Bump contact for semi-conductor devices.
Orthorhombic MnP struct.
Gallium compd. with gallium* (*1:2*), *11Cl [12044-77-8]
Digallium gold. Gallium gold (*Ga_2Au*)
$AuGa_2$ M 336.4
Fluorite struct.
***Gallium compd. with gold* (*7:2*)** [59977-57-0]
Heptagallium digold
Au_2Ga_7 M 881.9
Wyckoff, R.W.G., *Crystal Structures*, Interscience, N.Y., 1963, **1**, 128, 241 (*cryst struct*)
Zeng, X.F. *et al*, *Mater. Res. Soc. Symp. Proc.*, 1982, **10**, 213 (*solid state interfacial film formn*)
Grovenor, C.R.M. *et al*, *Thin Solid Films*, 1983, **104**, 409 (*interfacial reactions*)
Zeng, X.F. *et al*, *Solid-State Electron.*, 1984, **27**, 339 (*x-ray diffraction of contacts*)
Yoshie, T. *et al*, *Thin Solid Films*, 1984, **111**, 149 (*interfacial reactions*)
Chung, D.D.L. *et al*, *Thin Solid Films*, 1985, **128**, 299 (*formn at interfaces*)
Kim, T. *et al*, *Mater. Res. Soc. Symp. Proc.*, 1986, **54**, 437 (*interfacial effects in thin films*)

[AuGe] **IC-000702**
Germanium-gold system
Gold germanium
Alloy with two main phases.
***Germanium compd. with gold* (*1:3*)** [83231-92-9]
Germanium trigold. Gold germanium (*Au_3Ge*)
Au_3Ge M 663.5
Germanium compd. with gold* (*1:1*), *11Cl [12256-41-6]
Germanium gold. Gold germanium (*AuGe*)
AuGe M 269.5
Metals Handbook, *8th Ed.*, 1973, **8**, 267 (*phase diagram*)
Perfetti, P. *et al*, *J. Vac. Sci. Technol.*, 1982, **2**, 628 (*band struct*)
Kim, J. *et al*, *J. Vac. Sci. Technol.*, 1986, **4**, 762 (*compd formn at interfaces*)

$AuGeLi_2$ **IC-000703**
Gold lithium germanide ($AuLi_2Ge$)
Germanium gold dilithium. Germanium compd. with gold and lithium (1:1:2). Germanium gold lithium (*$GeAuLi_2$*). *Lithium gold germanide* (*Li_2AuGe*)
[12322-52-0]

Li_2AuGe

M 283.4

Alloy. Struct. related to NaTl-type. Possesses fcc lattice. Yellowish orange cryst., stable to dry air.
Pauly, H. *et al*, *Z. Metallk.*, 1968, **59**, 47 (*synth, cryst struct*)
Guetlich, P. *et al*, *J. Phys. Chem. Solids*, 1976, **37**, 1011 (*mössbauer*)

IC-000704

[AuGeNa]
Germanium-gold-sodium system
Alloy with two main phases.
Germanium compd. with gold and sodium* (*1:3:1*), *10Cl
[76327-19-0]
Germanium gold sodium (*$GeAu_3Na$*). *Germanium trigold sodium. Gold sodium germanide* (*Au_3NaGe*)
Au_3GeNa M 686.4
Cubic containing 16-coordinate Na, 12 coordinate Au and 9 coordinate Ge.
Germanium compd. with gold and sodium* (*1:1:2*), *10Cl
[57673-56-0]
Germanium gold sodium (*$GeAuNa_2$*). *Gold sodium germanide* (*$AuNa_2Ge$*). *Gold disodium germanide*
$AuGeNa_2$ M 315.5
Orthorhombic.
Wrobel, G. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **432**, 95 (*cryst struct*)
Doring, W. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1482 (*cryst struct*)

IC-000705

$AuH_4O_4^\ominus$
Tetrahydroxyaurate(*III*)(1−)
Aurate (*$Au(OH)_4^\ominus$*)
[73615-37-9]

$[Au(OH_4)]^\ominus$ (sq. pl.)

M 264.9 (ion)
Has photographic uses.
K salt: [88334-21-8].
AuH_4KO_4 M 304.0
Amorphous solid.
Ba salt (2:1): [93611-85-9].
$Au_2BaH_8O_8$ M 667.3
Amorphous solid.
Sr salt (2:1): [93611-84-8].
$Au_2H_8O_8Sr$ M 617.6
Pale yellow rectangular prisms.
Jander, G. *et al*, *Z. Anorg. Allg. Chem.*, 1960, **304**, 165 (*synth*)
Eur. Pat., 93 002, (1983); *CA*, **100**, 94460h.
Jones, P.G. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 1776 (*cryst struct*)

$AuH_{12}N_4^{3\oplus}$ **IC-000706**
Tetraamminegold(3+), 9Cl
[43739-93-1]

$[Au(NH_3)_4]^{3\oplus}$

M 265.0 (ion)
Monomethyldocosylphosphonate salt: [53934-39-7].
Antiwear additive for lubricating oils.
Trinitrate: [60117-73-9].
Colourless cryst. Sol. NH_4NO_3 soln. Dec. to metallic gold at *ca.* 230°.
Skibsted, L.H. *et al*, *Acta Chem. Scand., Ser. A*, 1974, **28**, 740, 764 (*synth, electrochem*)
Weishaupt, H. *et al*, *Z. Naturforsch., B*, 1976, **31**, 554 (*cryst struct*)
Alix, A.J.P. *et al*, *C.R. Conf. Int. Spectrosc. Raman: 7th*, *1980*, 1980, 211; *CA*, 1981, **94**, 111815e (*ir, raman*)
Manfait, M. *et al*, *Inorg. Chim. Acta*, 1981, **50**, 147 (*ir, raman*)

[AuHg]
Gold-mercury system **IC-000707**
Gold amalgam
Alloy with two main phases.
***Gold compd. with mercury* (*3:1*)**
Trigold mercury
Au_3Hg M 791.4
***Gold compd. with mercury* (*2:1*)** [12271-87-3]
Digold mercury
Au_2Hg M 594.5
White or grey metallic grains.
Atanasov, V. *et al*, *Dokl. Bolg. Akad. Nauk*, 1983, **36**, 465; *CA*, **99**, 108277d (*synth*)
Nechaev, S.V. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1986, **289**, 1483 (*x-ray diffraction*)

AuI **IC-000708**
Gold(*I*) iodide (AuI), 10Cl
[10294-31-2]

AuI

M 323.8
Struct. comprises zig-zag chain of linear gold(*I*) moieties. A mixed conductor-electrical conductor up to 0° and an ion conductor above this temp. Commercially available. Mp 100° dec.
Weiss, A. *et al*, *Z. Naturforsch., B*, 1956, **11**, 604 (*synth, cryst struct*)
Jagodzinski, H. *et al*, *Z. Kristallogr.*, 1959, **112**, 80 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1014 (*synth*)
Janssen, E.M.W. *et al*, *J. Less-Common Met.*, 1978, **59**, P65 (*phase diagram*)
Teicher, M. *et al*, *Phys. Rev. B: Condens. Matter*, 1978, **18**, 7134 (*elect cond*)

AuI_3 **IC-000709**
Gold(*III*) iodide (AuI_3), 9Cl
Auric iodide
[31032-13-0]

AuI_3

M 577.6
Not known to exist. 19th century references to dark-green, insol. AuI_3 are incorrect; the products obtained probably consisted of mixts. of AuI or complex iodides and salts of $I_3^\ominus$.
Ryan, J.L., *Inorg. Chem.*, 1969, **8**, 2058 (*existence*)

[AuIn] **IC-000710**
Gold-indium system
Indium gold
Several phases known, the most important detailed below.
***Gold compd. with indium* (*4:1*)** [63705-68-0]
Tetragold indium
Au_4In M 902.6
Hexagonal.
***Gold compd. with indium* (*3:1*)** [12598-23-1]
Au_3In M 705.7
Gold compd. with indium* (*9:4*), *10Cl [56320-57-1]
Nonagold tetraindium
Au_9In_4 M 2231.9
Cubic isostructural with Al_4Cu_9, γ-brass structure consists of 26 atom clusters.
***Gold compd. with indium* (*2:1*)** [55891-90-2]
Digold indium

Au_4In M 508.7
Orthorhombic

***Gold compd. with indium** (3:2)* [12598-24-2]
Trigold diindium
Au_3In_2 M 820.5

***Gold compd. with indium** (1:1)* [12006-55-2]
Gold indium
AuIn M 311.7
Tricline. Used in electrical contacts in microcircuits.

***Gold compd. with indium** (1:2)* [12044-81-4]
Gold diindium
$AuIn_2$ M 426.6
Cubic. Important in Josephson junction fabrication.

Hiscocks, S.E.R. *et al*, *Proc. R. Soc. London, Ser A*, 1964, **282**, 318 (*phase diagram*)
Metals Handbook, 8th Ed., 1973, **8**, 266 (*phase diagram*)
Brandon, J.K. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 527 (*cryst struct, Au_2In_3*)
Vandenberg, J.M. *et al*, *J. Appl. Phys.*, 1982, **53**, 7385 (*films, Au_2In_3*)
U.S. Pat., 258 157, (1982); *CA*, **96**, 172879s (*use, AuIn*)
Sinha, V. *et al*, *J. Less-Common Met.*, 1983, **95**, 259 (*formn, AuIn, $AuIn_2$*)
Goral, J.P. *et al*, *Ultramicroscopy*, 1985, **18**, 275 (*electron microsc, Au_2In*)
Marinković, Z. *et al*, *J. Less-Common Met.*, 1986, **115**, 225 (*compound formn*)
Goral, J.P. *et al*, *J. Less-Common Met.*, 1986, **116**, 63 (*phase diagram, electron microsc*)

AuInLa IC-000711
Gold compd. with indium and lanthanum (1:1:1), 10Cl
Gold indium lanthanum (AuInLa)
[60616-34-4]

AuLaIn

M 458.6
Alloy with Fe_2P struct.
Rossi, D. *et al*, *Z. Metallk.*, 1977, **68**, 493 (*cryst struct*)

AuK IC-000712
Gold potassium
Gold compd. with potassium (1:1), 10Cl
[51434-62-9]

AuK

M 236.0
Alloy. Solid with metallic lustre.
Kienast, G. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **310**, 143 (*phase diagram*)
Burns, R.C. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 2627 (*synth, reactions*)
Batchelor, R.J. *et al*, *Hyperfine Interact.*, 1986, **28**, 955 (*mössbauer*)
Batchelor, R.J. *et al*, *Inorg. Chem.*, 1986, **25**, 2009 (*synth, mössbauer, reactions*)

AuK_2Sb IC-000713
Gold potassium antimonide (AuK_2Sb)
Antimony compd. with gold and potassium, 10Cl. Antimony gold potassium (SbAuK$_2$)
[75228-62-5]

AuK_2Sb

M 396.9
Isostructural with $AsCuNa_2$ struct. type. Cryst.
Muss, C. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1055 (*cryst struct*)

AuLi IC-000714
Gold lithium
Gold compd. with lithium (1:1), 10Cl
[12370-48-8]

AuLi

M 203.9
Alloy. Solid with metallic lustre.
Kienast, G. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **310**, 143 (*phase diagram*)
Ihle, H.R. *et al*, *J. Chem. Phys.*, 1977, **66**, 5105 (*matrix study*)
Stone, H.E.N. *et al*, *Acta Metall.*, 1978, **26**, 1399 (*rev*)
Batchelor, R.J. *et al*, *Inorg. Chem.*, 1986, **25**, 2009 (*synth, mössbauer*)

AuLiMgSn IC-000715
Gold lithium magnesium tin (AuLiMgSn)
Gold compd. with lithium, magnesium and tin, 10Cl
[76327-17-8]

AuLiMgSn

M 346.9
Alloy. $CuHg_2Ti$ struct. type. Cryst.
Eberz, U. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1341 (*cryst struct*)

$AuLi_2Sn$ IC-000716
Gold lithium tin ($AuLi_2Sn$)
Gold compd. with lithium and tin (1:2:1), 10Cl
[12044-82-5]

$AuLi_2Sn$

M 329.5
Alloy. $CuHg_2Ti$ struct. type. Cryst.
Guetlich, P. *et al*, *J. Phys. Chem.*, 1976, **37**, 1011 (*mössbauer*)
Eberz, U. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1341 (*cryst struct*)

[AuMg] IC-000717
Gold-magnesium system
Series of alloys.

Gold compd. with magnesium (4:1) [12256-75-6]
Tetragold magnesium
Au_4Mg M 812.1
Cu_3Pd struct. type, monoclinic. Also complicated $Au_{77}Mg_{23}$ struct.

Gold compd. with magnesium (3:1) [12044-97-2]
Digold magnesium
Au_2Mg M 418.2

Gold compd. with magnesium (1:1) [12256-45-0]
AuMg M 221.2
CsCl structure type.

Gold compd. with magnesium (1:2) [12399-98-3]
$AuMg_2$ M 245.5
Superstructure of Co_2Si struct. kind.

Gold compd. with magnesium (1:3) [12399-99-4]
Gold trimagnesium
$AuMg_3$ M 269.8
Superstruct. of Na_3As kind.

Brauer, G. *et al*, *Z. Phys. Chem.*, 1936, **33**, 304 (*cryst struct, AuMg*)
Terasaki, O. *et al*, *J. Appl. Crystallogr.*, 1982, **15**, 65 (*cryst struct, Au_3Mg*)
Van Tandeloog, G. *et al*, *Phys. Status Solidi A*, 1982, **69**, 103 (*cryst struct, Au_4Mg*)
Abouchacra, G. *et al*, *Radiat. Eff.*, 1982, **64**, 189 (*synth, cryst struct, Au_3Mg*)

Bonsov, Yu.A. *et al*, *Zh. Struki. Khim.*, 1983, **24**, 97 (*theory*)
Daams, J.L.C. *et al*, *Philips J. Res.*, 1984, **39**, 275 (*cryst struct, $AuMg_2$, $AuMg_3$*)
Chulkov, E.V. *et al*, *Piz. Met. Metalloved.*, 1985, **59**, 730; *CA*, **102**, 224448q (*theory*)

AuMgSb IC-000718
Gold magnesium antimonide (AuMgSb)
Antimony compd. with gold and magnesium(1:1). Antimony gold magnesium (SbAuMg)
[101360-62-7]

AuMgSb

M 343.0
Characterised as ternary 'Zintl phase' with a filled zinc blende struct.
Eberz, U. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1341 (*synth, cryst struct*)
Pulm, H. *et al*, *J. Less-Common Met.*, 1986, **115**, 127 (*pe, aes*)

AuMgSn IC-000719
Gold magnesium tin (AuMgSn)
Gold compd. with magnesium and tin (1:1), 11Cl
[76327-16-7]

AuMgSn

M 339.9
Alloy. Cubic AlGeLi struct. type.
Eberz, U. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1341 (*cryst struct*)

$AuN_4O_{12}^{\ominus}$ IC-000720
Tetrakis(nitrato-*O*)aurate(*III*)(1 −), 9Cl
Tetranitratoaurate(III)(*1 −*)

$Au(ONO_2)_4^{\ominus}$

M 444.9 (ion)
Unusual unidentate nitrate groups; square planar. Synth. by reaction between N_2O_5 and $AuX_4^{\ominus}$ at −78°.
Nitronium salt: Fairly unstable, v. moisture-sensitive large yellow cryst. (conc. HNO_3). V. sol. $MeNO_2$, fuming HNO_3. Sl. dec. under dry N_2; rapid dec. in moist air, evolving white fumes. Dec. sl. in $MeNO_2$ soln., forming a gold mirror.
▷ Reacts explosively with DMSO and Me_2CO.
Na salt: [38139-24-1].
Synth. from nitronium salt. V. unstable cryst. (conc. HNO_3).
K salt: [23451-05-0].
Hygroscopic pale yellow cryst. (HNO_3). Diamagnetic.
Rb salt: [38139-26-3].
Cryst. (conc. HNO_3).
Cs salt: [38139-27-4].
Fairly stable cryst. (conc. HNO_3).
Garner, C.D. *et al*, *J. Chem. Soc. A*, 1970, 3092 (*synth, cryst struct*)
Addison, C.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1440 (*synth, ir, raman*)

$AuN_{12}^{\ominus}$ IC-000721
Tetra(azido)aurate(1 −), 11Cl

$[Au(N_3)_4]^{\ominus}$

M 365.0 (ion)
▷ Potentially explosive.
Ph_4As salt: [14781-43-2].
Colourless cryst. (CH_2Cl_2/pet. ether). Mp 127°.
Beck, W. *et al*, *Chem. Ber.*, 1967, **100**, 2335; 1984, **117**, 419 (*synth, cryst struct*)

AuNa IC-000722
Gold sodium (AuNa)
Gold compd. with sodium (1:1), 10Cl
[61115-29-5]

AuNa

M 219.9
Alloy. Solid with metallic lustre.
Kienast, G. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **310**, 143 (*phase diagram*)
Piacenti, V. *et al*, *High Temp. Sci.*, 1977, **9**, 189 (*gas phase thermodyn*)
Batchelor, R.J. *et al*, *Inorg. Chem.*, 1986, **25**, 2009 (*synth, mössbauer*)

[AuNaSi] IC-000723
Gold-sodium-silicide system

***Gold sodium silicide** (Au$_3$NaSi)* [76328-83-1]
Trigold sodium silicide
Au_3NaSi M 641.9
Cubic, with containing 16-coordinate Na, 12 coordinate Au and 9 coordinate Si.

***Gold sodium silicide** ($Au_2Na_{1.5}Si$)*
$Au_2Na_{1.5}Si$ M 456.5
Cell contents $Au_{81}Na_{52}Si_{20}$. Cubic $Mg_{32}(ZnAl)_{49}$ struct. type.
Döring, W. *et al*, *Z. Naturforsch., B*, 1979, **34**, 1715; 1980, **35**, 1482 (*cryst struct*)

[AuNaSn] IC-000724
Gold-sodium-tin system
Alloy series.

***Gold compd. with sodium and tin** (3:2:1), 11Cl*
Au_3Na_2Sn M 755.5
Cubic $Mg_{32}(ZnAl)_{49}$ struct. type. Cell contents $Au_{78}Na_{60}Sn_4$.

***Gold sodium tin** (AuNaSn)* [57673-57-1]
Gold compd. with sodium and tin (1:1:1), 10Cl
AuNaSn M 338.6
Orthorhombic (E-phase, NiSiTi struct. type).
Wrobel, G. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **432**, 95 (*cryst struct, AuNaSn*)
Döring, W. *et al*, *Z. Naturforsch., B*, 1979, **34**, 1715 (*cryst struct, Au_3Na_2Sn*)

$AuO_2^{\ominus}$ IC-000725
Dioxoaurate(1 −)

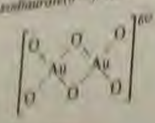
$[AuO_2]^{\ominus}$

M 228.9 (ion)
K salt: [12446-76-3]. *Gold potassium oxide, 8Cl*
$AuKO_2$ M 268.0
Catalyst for oxidation of aldehydes to carboxylic acids.
Sl. moisture-sensitive yellow cryst. Dec. slowly in air. Dec. *ca.* 450°, forming metallic gold.
Rb salt: [12512-20-8]. *Gold rubidium oxide, 8Cl*
AuO_2Rb M 314.4
Moisture-sensitive yellow solid. Dec. *ca.* 500°.
Hoppe, R. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **314**, 4 (*synth, props*)

South African Pat. 0 802 009, (1968); *CA*, 1969, **70**, 87631v (*synth*)
Wassel-Nielsen, H.-D. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **375**, 43 (*synth, cryst struct*)

IC-000726

AuO_5^{3G}
Trioxoaurate(*III*)(3−)
Dioxo-μ-oxido-trioxodiaurate(6−). Aurate ($Au_2O_5^{3G}$)



dimer

M 344.9 (ion)
Dimeric, planar struct.
Dimer, hexa-Na salt [80424-36-8] *Gold sodium oxide* ($Au_2Na_6O_5$)
$Au_2Na_6O_5$ M 627.8
Deliquescent golden yellow transparent cryst.

[12312-19-9]
Hoppe, R. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **324**, 4 (*synth*)
Klassen, H. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1395 (*synth, props, cond struct*)

$AuO_2S_2^{3G}$ **IC-000727**
Bis(thiosulfato)aurate(*I*)(3−)
Bis(monothiosulfato(2−)-O,S)aurate(1−)

$[Au(SSO_3)_2]^{3G}$

M 421.2 (ion)
Tri-Na salt, monohydrate [15283-43-1]. *Sodium aurothiosulfate. Aurothiosulfate. Aurosan. Aurothion. Auracidine. Aurolin. Auropax. Ausopin. Sanochrysine. Crysalbine. Crysion. Nasserstein. Sulfhercisol. Thiochrysine*
$AuH_2Na_2O_5S_4$ M 508.2
Antirheumatoid drug. Lowers blood pressure by inhibiting prostaglandin synthesis. Chemical sensitiser of photographic AgBr films. Light-sensitive glistening white cryst. Aq. solns dec. on standing. Sol. H_2O, insol. EtOH, org. solvs. Centrosymmetric dimer with Au···Au 330 pm. Coord. about gold is linear with thiosulfate S-bonded. Dehydrates at 120°

[15843-98-3]

Baggio, R.F. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 3191 (*cryst struct, str*)
Baltzer, B. *et al*, *Inorg. Chem.*, 1978, **13**, 1836 (*synth, cryst struct*)
Gettler, P.T., *Script. Bonding (Berlin)*, 1976, **27**, 171 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **23**, 398 (*rev*)
Mazid, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1980, 1261 (*cryst*)
Davidson, G. *et al*, *Spectrochimica*, 1981, **37**, 81 (*vibration spectra in soln, struct*)
Brown, K. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4935 (*Mössbauer*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 729?
Merck Index, 11th Ed., 1989, 8422

[AuPb]
Gold-lead system **IC-000728**
Alloy series

Gold compd. with lead *(2:1)*, *10CI* [12006-66-5]
Au_2Pb M 601.1
Congruent in peritectic reaction at 434°. Stable at >209°. Fm Cu_2Mg type struct.

Gold compd. with lead *(1:1)* [12256-51-8]
AuPb M 404.1
Generated in peritectic reaction at 221.5°.

Gold compd. with lead *(1:2), HCI* [12006-57-4]
$AuPb_2$ M 611.3
Generated in peritectic reaction at 253°. Tetragonal Al_2Cu type.

Wollbaum, H., *Z. Metallk.*, 1943, **35**, 218 (*cryst struct*)
Smithells Metals Handbook, 8th Ed., 1973, **8**, 244, 268 (*cryst struct, phase diagram*)
Evans, D.S. *et al*, *Mater. Res. Soc. Symp. Proc.*, 1983, **19**, 383 (*phase diagram*)

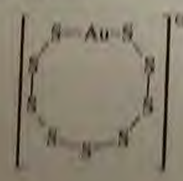
AuRb **IC-000729**
Gold rubidium (AuRb)
Gold compd. with rubidium (1:1)
[12512-22-0]

AuRb

M 282.4
Alloy with CsCl struct. type. Yellow brown to bronze metal.

Kienast, G. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **310**, 143 (*phase diagram*)
Tinelli, G.A. *et al*, *J. Solid State Chem.*, 1978, **25**, 157 (*cryst struct, nmr*)
Busse, B. *et al*, *Ber. Bungenges. Phys. Chem.*, 1981, **85**, 309 (*gas phase dimer*)
Batchelor, R.J. *et al*, *Hyperfine Interact.*, 1986, **28**, 1055 (*mössbauer*)
Batchelor, R.J. *et al*, *Inorg. Chem.*, 1986, **25**, 2009 (*synth, mössbauer*)

AuS_9^{4G} **IC-000730**
Nonathiosaurate(1−), 11CI



M 485.3 (ion)
Puckered ring with linear S—Au—S.
Ph_4As salt [88867-22-5].
Synth. from $Au(SCN)_2^{4G}$ and Ph_4AsS_2 in EtOH. Air- and light-stable bright yellow platelets (EtOH). Sol. DMSO; insol. H_2O, other org. solvs. Dec. in acid.

Maebach, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 246 (*synth, ir, cryst struct*)

$AuSb^{1G}$ **IC-000731**
Stibidosaurate(2−)

$[AuSb]^{1G}$

M 318.7 (ion)
Struct. comprises infinite zig-zag chains resembling gold(*I*) halides. The gold atoms have linear co-ordination geometries.
Di-Na salt [75228-61-4]. *Antimony gold sodium (1/1/2), 5Sb,Au,Na3-Antimony compd. with gold and sodium (1:1:2), 10CI*
$AuNa_2Sb$ M 364.6
Orthorhombic cryst.

Mun, C. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1055 (*synth, cryst struct*)

$AuSb_2$ **IC-000732**
Aurostibite, 11CI
Gold diantimonide. Antimony gold (Sb_2Au)
[12044-89-2]

$AuSb_2$

M 440.4
Alloy with cubic FeS_2 struct. Mineral from NW Territories, Canada, Yugoslavia and elsewhere. Metal. Cryst. resembling galena.

[12044-88-1]
Smithells Metals Handbook, 8th Ed., 1973, **8**, 243, 268 (*cryst struct, phase diagram*)
Simic, V. *et al*, *J. Less-Common Met.*, 1983, **95**, 259 (*formn at interfaces*)
Kulichikhina, R.D., *Mineral. Rudn. Mestorozhd.*, 1983, 104; *CA*, **100**, 106770z (*optical props*)
Nekrasov, I.Ya. *et al*, *Mineral. Zh.*, 1985, **7**, 61; *CA*, **103**, 126617c (*synth*)

$AuSb_6Te$ **IC-000733**
Antimony gold telluride (Sb_6AuTe), 11CI
Hexaantimony gold tellurium
[92522-32-2]

$AuSb_6Te$

M 1055.0
High temp. bulk phase which crystallizes in a cubic α—Po struct. Semiconductor.

Shanov, V. *et al*, *Mater. Res. Soc. Symp. Proc.*, 1984, **22**, 351 (*synth*)

AuSe **IC-000734**
Gold selenide, 10CI
[23331-11-3]

$Au^{I}Au^{III}Se_2$

M 275.9
Mixed valence compd. Linear Au(*I*) and square planar Au(*III*) fragments form infinite rods. Coordination formula is $[Au^{II}Se_{2/1}Au^{III}Se_{4/1}]$. Black thin needles or plates.

Cranton, G.E. *et al*, *Can. J. Chem.*, 1968, **46**, 2637 (*synth, phase diagram*)
Rabenau, A. *et al*, *J. Less-Common Met.*, 1971, **24**, 291; 1976, **48**, 89 (*synth, cryst struct*)
Srivastava, M.M. *et al*, *Z. Metallk.*, 1971, **62**, 641 (*ed*)
Bacon, S. *et al*, *Lab. Pract.*, 1977, **26**, 867 (*anal*)

[AuSn] **IC-000735**
Gold-tin system
A series of alloys

Gold compd. with tin *(5:1), 10CI* [12006-74-5]
Pentagold tin
Au_5Sn M 1103.5
Rhombohedral R3 superstructure of the hcp structure.

Gold compd. with tin *(2:1)* [57142-94-6]
Digold tin
Au_2Sn M 512.6
Atomization energy 540.5 kJ mol^{-1}. ΔH_f° 493.0 kJ mol^{-1}

Gold compd. with tin *(1:1), HCI* [12006-66-9]
AuSn M 315.6
Hexagonal NiAs struct. ζ—AuSn hcp magnesium struct.

Gold compd. with tin *(2:3)* [57142-95-7]
Au_2Sn_3 M 631.3
Atomization energy 726 kJ mol^{-1}. ΔH_f° 610 kJ mol^{-1}.

Gold compd. with tin *(1:2)* [12256-54-1]
Gold ditin
$AuSn_2$ M 434.3
Orthorhombic.

Gold compd. with tin *(1:3)* [57142-93-5]
Gold tritin
$AuSn_3$ M 553.0
Atomization energy 788 kJ mol^{-1}. ΔH_f° 477 kJ mol^{-1}.

Gold compd. with tin *(1:4)* [12044-91-6]
Gold tetratin
$AuSn_4$ M 671.8
Face centred orthorhombic struct.

Davies, H.A. *et al*, *J. Inst. Met.*, 1968, **96**, 220 (ζ-*phase, AuSn*)
Smithells Metals Handbook, 8th Ed., 1973, **8**, 244, 269 (*cryst struct, AuSn, $AuSn_2$, $AuSn_4$, phase diagram*)
Osada, K. *et al*, *Trans. Jpn. Inst. Metals*, 1974, **15**, 256 (*cryst struct, Au_5Sn*)
Simic, V. *et al*, *J. Less-Common Met.*, 1977, **51**, 177 (*thin films, Au_5Sn*)
Kubiak, R. *et al*, *J. Less-Common Met.*, 1984, **97**, 285 (*cryst struct, $AuSn_4$*)
Kingcade, J.E. *et al*, *J. Chem. Phys.*, 1986, **84**, 3452 (*gas phase clusters*)
Tanaka, T. *et al*, *Nippon Kessho Gakkaishi*, 1986, **28**, 523; *CA*, **105**, 87979 (*mössbauer, AuSn, $AuSn_4$*)

[AuSr] **IC-000736**
Gold-strontium system
Alloy with two main phases.

Gold compd. with strontium *(1:1), HCI* [88121-13-5]
AuSr M 284.5
Monoclinic Struct. related to FeB-CrB type. Each gold surrounded by a trigonal prism of Sr atoms tricapped by one Sr and two Au.

Gold compd. with strontium *(2:3), HCI* [102678-02-4]
Digold tristrontium
Au_2Sr_3 M 656.7
Er_2Ni_3 structural type.

Borisov, Yu.A. *et al*, *Zh. Strukt. Khim.*, 1983, **24**, 97 (*theory, AuSr*)
Fornasini, M.L. *et al*, *J. Solid State Chem.*, 1985, **59**, 66 (*cryst struct, synth; AuSr*)
Fornasini, M.L. *et al*, *Rev. Chim. Miner.*, 1986, **23**, 791 (*cryst struct, Au_2Sr_3*)

$AuTe_2$ **IC-000737**
Gold tellurides ($AuTe_2$), 9CI
Gold ditelluride
[12006-61-0]

$AuTe_2$

M 452.1
Struct. comprises $AuTe_2$ molecules with additional weaker Au···Te interactions.

Mineral-form
Calaverite
Occurs widely in low to high temp. vein deposits, commonly associated with other minerals. Brass yellow to silver white monoclinic cryst.

Mineral-form
Krennerite
Occurs mainly in low temp. veins at sites in U.S.A., Canada, Transylvania, Australia and Fiji. Silver white to pale yellowish white, orthorhombic cryst. Metallic

[1303-56-6, 56499-48-0]

Tunnel, G. *et al*, *Am. Mineral.*, 1950, **35**, 959 (*cryst struct*)
Raoot, S. *et al*, *Lab. Pract.*, 1977, **26**, 867 (*anal*)
Sham, T.K. *et al*, *Phys. Rev. B: Condens. Matter*, 1979, **19**, 539 (*mössbauer*)

IC-000738

[AuZn]

Gold-zinc system

Three alloys.

Gold compd. with zinc *(3:1)* [12256-74-5]
Trigold zinc
Exists in three cryst. modifications.

Gold compd. with zinc *(1:1), 11CI* [12006-63-2]
AuZn M 262.3
Ordered bcc struct. based on CsCl. Cryst.

Gold compd. with zinc *(1:3), 11CI* [11089-97-7]
Gold trizinc
$AuZn_3$ M 393.1
High temp. form ordered bcc CsCl (γ_1). Low temp. form ordered cubic

Smithells Metals Handbook, 5th Ed., 1973, **8**, 244, 269 (*cryst struct, phase diagram*)
Trulio, J. *et al*, *J. Phys. F*, 1982, **12**, 2165 (*domain struct., Au_3Zn*)
Ingles, H. *et al*, *Monatsh. Chem.*, 1983, **114**, 1177 (*congruent mp*)
Simic, V. *et al*, *Nauchno-Teh. Pregl.*, 1983, **33**, 42; *CA*, 1984, **100**, 72816m (*intermetallic forms in thin films*)
Stearns, R. *et al*, *Phys. Status Solidi B*, 1985, **129**, 735 (*optical prop.*)

Au_2Bi IC-000739

Bismuth gold ($BiAu_2$)
Maldonite, 11CI *Digold bismuth*

[12426-53-8]

Au_2Bi

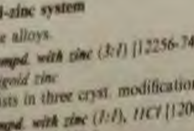
M 682.9
β-phase has face centred cubic Cu_2Mg struct. Mineral. Light cinammon cream-coloured in reflected light.

Mineral. Handbook, 5th Ed., 1971, **3**, 244, 266 (*cryst. struct, phase diagram*)
Nakazawa, I.Ya. *et al*, *Mineral. Zh.*, 1985, **7**, 82; *CA*, **103**, 128617 (*mineral forms*)

$Au_2F_{10}O_2Te_2$ IC-000740

Hexakis(pentafluorohydroxytellurato)digold(*III*)
Bis[μ-(pentafluorohydroxytellurato-O:O)]tetrakis(pentafluorohydroxytellurato-O)digold(III), 11CI
Gold(III) pentafluorohydroxytellurate dimer

[67972-82-4]



M 1025.4
Struct. analogous to Au_2Cl_6 but dihedral angle of 34° between two square planes. Synth. from AuF_3 and $B(OTeF_5)_3$. Stable brown-orange cryst. (by subl.), sensitive to hydrol. Mp 128°. Subl.$_{0.75}$ 110°

Huppmann, P. *et al*, *Z. anorg. Allg. Chem.*, 1985, **524**, 26 (*cryst. struct, raman, F-19 nmr, ms*)

Au_2Ge_2Sr IC-000741

Germanium compd. with gold and strontium (2:2:1), 9CI
Germanium gold strontium (Ge_2Au_2Sr). Digermanium digold strontium

[37248-67-2]

$SrAu_2Ge_2$

M 626.7
Alloy. Tetragonal $ThCr_2Si_2$ struct. type.

May, N. *et al*, *Z. Naturforsch., B*, 1972, **27**, 864 (*cryst struct*)

Au_2Ge_2Th IC-000742

Gold thorium germanide (2:1:2)
Digold thorium digermanide. Germanium gold thorium (Ge_2Au_2Th)

$ThAu_2Ge_2$

M 771.1
Alloy. $ThCu_2Si_2$ struct.

Marazza, R. *et al*, *J. Less-Common Met.*, 1978, **53**, 193 (*cryst struct*)

$Au_2I_{10}Tl_6$ IC-000743

Gold thallium iodide ($Au_2Tl_6I_{10}$), 10CI
Digold hexathallium decaiodide

[67338-07-2]

$Au_2Tl_6I_{10}$

M 2889.2
Struct. comprises framework of Tl_6I_8 with channels parallel to *c*-axis. These channels contain $Au^{\oplus}$ with planar trigonal coordination, and $I_3^{\ominus}$ or $I^{\ominus}$ ions. Synth. in closed system. Used as battery electrodes. Black cryst. with golden lustre. Mp 276° dec. (sealed tube). Dec. at 65° *in vacuo* losing I_2.

Ger. Pat., 2 801 912, (1979); *CA*, **91**, 178133n (*use*)
Strieger, W. *et al*, *Z. Naturforsch., B*, 1979, **34**, 685 (*synth, cryst struct*)
Stoltz, H.J. *et al*, *Z. Naturforsch., A*, 1980, **35**, 389 (*raman, ir*)

Au_2O_3 IC-000744

Gold(*III*) oxide (Au_2O_3), 10CI
Digold trioxide

[1303-58-8]

Au_2O_3

M 441.9
Polymeric struct. based on square planar gold atoms. The oxygen atoms are either coordinated to two or three gold atoms. Synth. from Au_2O_3 aq. in $HClO_4$ after heating in a quartz tube. Commercially available. Ruby orthorhombic cryst. Studied on gold surfaces involved in electrochemical oxidation process.

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1015 (*synth*)
Lolurupel, M.M. *et al*, *Electrochim. Acta*, 1976, **21**, 957 (*electrochem*)
Schwarzmann, E. *et al*, *Z. Naturforsch., B*, 1976, **31**, 135 (*synth, struct*)
Jones, P.G. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 1435 (*cryst struct*)

$Au_2O_7Se_2$ IC-000745

Gold oxide selenite ($Au_2O(SeO_3)_2$)
μ-Oxobis[selenito(2−)-O]digold

[85025-30-5]

$Au_2(SeO_3)_2O$

M 663.8
Layer structure involving selenite and oxide anions. Synth. by reaction of gold and selenic acid in a sealed tube at 280°. Air-stable red transparent platelets.

Jones, P.G. *et al*, *Z. Naturforsch., B*, 1983, **38**, 10 (*synth, cryst struct*)

$Au_2O_{11}Se_4$ IC-000746

Gold diselenite selenite, 11CI
Digold(III) bis(selenite) diselenite

[81627-23-8]

$Au_2(SeO_3)_2(Se_2O_5)$

M 885.7
Originally formulated as $[Au_2(SeO_4)_3]$. Struct. contains three cross-linked chains of the form [...Au-(selenite or diselenite)-Au...]. Synth. by reaction of gold metal and selenic acid at 280°. Used to colour glasses. Yellow cryst.

Jones, P.G. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1050 (*synth, cryst struct*)

Au_2P_3 IC-000747

Gold phosphide (Au_2P_3), 10CI
Digold triphosphide

[12044-95-0]

M 486.8
Struct. comprises $P_6^{4\ominus}$ rings linked directly and through Au(*I*) atoms. Obt. via chemical transport techniques. Metallic conductor. Cryst. Diamagnetic.

Haraldsen, H. *et al*, *Z. Elektrochem.*, 1931, **37**, 502 (*synth*)
Olofsson, O., *Acta Chem. Scand.*, 1970, **24**, 723 (*synth*)
Jeitschko, W. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 573 (*synth, cryst struct*)

Au_2S IC-000748

Gold(*I*) sulfide (Au_2S)
Aurous sulfide

[1303-60-2]

Au_2S

M 425.9
Prepd. from $K[Au(CN)_2]$ + H_2S. Commercially available. Black-brown powder when dry, steel-grey when moist. Prac. insol. H_2O. Mp 240° dec.

Hofmann, L. *et al*, *Ber.*, 1887, **20**, 2361 (*synth*)
Hirsch, H. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1966, **263**, 1328 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1016 (*synth*)
Merck Index, 11th Ed., 1989, No. 4417.

Au_2S_3 IC-000749

Gold(*III*) sulfide (Au_2S_3)
Auric sulfide

[1303-61-3]

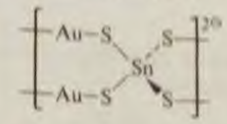
M 490.1 Au_2S_3

Prepd. from $LiAuCl_4$, $HAuCl_4$ or $AuCl_3$ with H_2S. Commercially available. Deep black solid. Insol. H_2O. Mp 197° dec.

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1017.
Merck Index, 11th Ed., 1989, No. 4432.

$Au_2S_4Sn^{2\ominus}$ IC-000750

(Tetrathiostannato)diaurate(2−)
Tetrathioxostannatediaurate(2−), 10CI

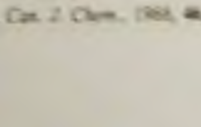


M 640.9 (ion)
Ba salt: [68879-44-7]. *Barium digold tetrathiostannate. Gold barium thiostannate. Barium gold tin sulfide ($BaAu_2SnS_4$)*
Au_2BaS_4Sn M 778.2
Obt. by heating binary sulfides at 400-540°. Red mosaic blocks. Orthorhombic. Chain struct. in solid state with Au—Au 298 pm.

Teske, C.L., *Z. Anorg. Allg. Chem.*, 1978, **445**, 193 (*cryst struct*)

$Au_2S_8^{2\ominus}$ IC-000751

Bis[μ-(tetrathio)]diaurate(2−), 11CI
Di-μ-tetrasulfidodiaurate(2−)



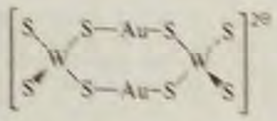
M 650.4 (ion)
Bis-Ph_4P salt: [90939-27-8].
Red-brown cryst.

Muller, A. *et al*, *Inorg. Chim. Acta*, 1984, **85**, L39 (*synth, cryst struct*)

$Au_2S_8W_2^{2\ominus}$ IC-000752

Bis(tetrathiotungstato)diaurate(2−)
Diauratetetra-μ-thioxotetrathioxoditungstate(2−), 9CI

[65015-83-0]



M 1018.1 (ion)
Interatomic distance Au—Au 311 pm.
Bis-Ph_4P salt: Dark red cryst. (DMF/EtOH).

Müller, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1978, **90**, 52 (*synth, cryst struct, ir, mössbauer*)
Strähle, J. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **456**, 241 (*synth*)

Au_2SeTe IC-000753

Gold selenide telluride (Au_2SeTe)
Digold selenide telluride

Au_2SeTe

M 600.4
Primitive orthorhombic cryst.

Cranton, G.E. *et al*, *Can. J. Chem.*, 1968, **46**, 2637 (*phase diagram, x-ray data*)

IC-000754

Au_2Si_2Th

Gold thorium silicide (Au_2Si_2Th)

Digold thorium disilicide

Au_2ThSi_2

M 482.1

$ThCu_2Si_2$ structure type. Solid.

Marazza, R. *et al*, *J. Less-Common Met.*, 1978, **53**, 193 (*cryst struct*)

IC-000755

Au_2Si_2U

Gold uranium silicide (Au_2USi_2)

Digold uranium disilicide

Au_2USi_2

M 688.1

$ThCu_2Si_2$ structure type. Solid.

Marazza, R. *et al*, *J. Less-Common Met.*, 1978, **53**, 193 (*cryst struct*)

IC-000756

$Au_3Sb_4Y_3$

Gold yttrium antimonide ($Au_3Y_3Sb_4$)

Antimony compd. with gold and yttrium (4:3:3)

Tetraantimony trigold triyttrium. Antimony gold yttrium ($Sb_4Au_3Y_3$)

[63144-21-8]

$Au_3Y_3Sb_4$

M 1344.6

Cubic. Y has four close Au neighbours and four close Sb neighbours. Alloy.

Daniel, A.E., *Acta Crystallogr., Sect. B*, 1977, **33**, 1579 (*cryst struct*)

IC-000757

Au_xSi

Gold silicide (Au_xSi)

Trigold silicide

[12588-93-1]

Au_xSi

M 618.9

Solid.

Metals Handbook, 8th Ed., 1973, **8**, 268 (*phase diagram*)

Bisi, O. *et al*, *J. Phys. C*, 1982, **15**, 4709 (*electronic struct*)

Johnson, A.A. *et al*, *Mater. Sci. Eng.*, 1983, **61**, 231 (*diffusion*)

Johnson, D.N. *et al*, *Solid-State Electron.*, 1984, **27**, 1107 (*surface coating*)

IC-000758

Au_2Cl_6

Tetra-μ-chlorotetrachlorotetraaurate, 10Cl

Octachlorotetraaurate

[62792-24-9]

$Au^I_2Au^{III}_2Cl_6$

M 1071.2

Mixed valence compd., square planar and linear fragments are linked to give polymeric struct. Synth. from Au_2Cl_4 and Cl-benzyltrichlorogold. IC-002272. Black cryst. chlorinated solvs. or $SOCl_2$.

Monomer: Dichlorogold Gold dichloride

$AuCl_2$ M 267.8

Dell'Amico, D.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1829 (*synth*)

Dell'Amico, D.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1977, 31 (*cryst struct*)

IC-000759

Au_4KSn_2

Gold potassium tin (Au_4KSn_2)

Gold compd. with potassium and tin (4:1:2), 10Cl

[68449-33-2]

Au_4KSn_2

M 1064.3

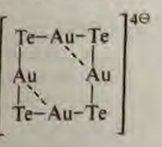
Alloy. Tetragonal struct. derived from Tl_2Se by removing two sites per cell.

Sinnen, H.-W. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1077 (*cryst struct*)

IC-000760

$Au_4Te_4^{4\ominus}$

Tetra-μ-telluroxotetra-*cyclo*-aurate(4 –), 11Cl



M 1298.2 (ion)

Di-K, bis-Ph_4P salt, tetrakis-ethylenediamine complex: [96211-81-3].

Synth. from KAuTe alloy, ethylenediamine and Ph_4PBr. Dark red cryst. The potassium cations are coordinated on opposite faces of $(AuTe)_4$ square.

Di-K, bis-Ph_4P salt, bis-DMF, bis-MeOH complex: [96211-83-5].

Dark red cryst.

Haushalter, R.C., *Angew. Chem., Int. Ed. Engl.*, 1985, **97**, 432 (*synth, cryst struct*)

IC-000761

Au_7IP_{10}

Gold iodide phosphide (Au_7IP_{10}), 10Cl

Iododecaphosphidoheptagold

[67116-00-1]

Au_7IP_{10}

M 1815.4

Struct. comprises infinite sheets of P_{12} rings containing 3-coordinate Au(*I*) atoms. The sheets are joined by linear P—Au—P and Au—I—Au bridges. Synth. from Au_2P_3 and 7 wt.% iodine in metal vapour transport reaction. Cryst. obt. by chemical transport from 697-647°. Diamagnetic. Metallic conductor.

Beck, C.G. *et al*, *Monatsh. Chem.*, 1972, **103**, 482 (*synth*)

Binnewies, M., *Z. Naturforsch., B*, 1978, **33**, 570 (*cryst struct*)

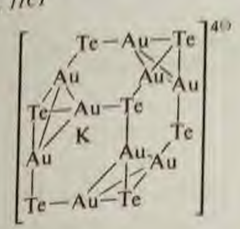
Jeitschko, W. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 573 (*synth, cryst struct*)

IC-000762

$Au_8KTe_7^{4\ominus}$

Heptatelluroxopotassatenonaaurate(4 –)

Tri-μ-telluroxotetra-μ$_3$-telluroxononaaurate(5 –) potassium(1+), 11Cl



M 2704.9 (ion)

K^+ shown, embedded in cluster. Struct. comprises cube of Te atoms with missing vertex. Gold atoms lie on remaining edges.

Tetrakis-Ph_4P salt: [96211-78-8].

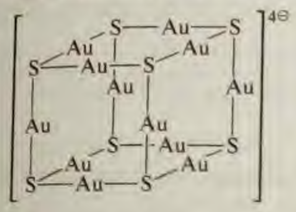
Synth. from K_3AuTe_2 alloy and Ph_4PBr in MeOH. Red triangular plates (MeOH).

Haushalter, R.C. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1985, **97**, 412 (*synth, cryst struct*)

IC-000763

$Au_{12}S_8^{4\ominus}$

Octa-μ$_3$-thioxododecaaurate(4 –), 11Cl



M 2620.1 (ion)

Consists of cube of $S^{2\ominus}$ ligands with Au atoms along mid-points of edges.

Tetrakis-Ph_4As salt: [91742-15-3].

Light-sensitive, light yellow cryst. (H_2O). Sol. DMF, DMSO. Mp 230° dec.

Marbach, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 715 (*synth, cryst struct*)

IC-000764

B

Boron

[7440-42-8]

B

M 10.8

Atomic No. 5. Ground state electron config. $[He]2s^22p^1$. Discovered by L.J. Gay-Lussac, L.J. Thenard, and by Sir H. Davy in 1808. Obt. pure by Moissan in 1892. There are 6 known isotopes of which 2 are natural, and used (particularly ^{11}B) in nmr spectroscopy. Polymorphic, with cryst. and amorphous forms. Cryst. forms are extremely hard and refractory, with v. low electrical conductivity. Most abundant mineral is tourmaline, but most important source is borax, known to the ancient world. Element manuf. (1) by electrolysis of fused borates (2) by H_2 red. of volatile B compds. e.g. BBr_3. Also synth. by thermal dec. of B hydrides and halides. Metallurgical uses of pure element are rare. Alloys with other elements have widespread use (see individual borides). Essential for plant life. Cryst. B is v. unreactive; reacts with NaOH at 500°, Na_2CO_3 at 850°. Dissolves in H_2SO_4/HNO_3 (2:1). Amorphous B is v. reactive, sometimes violently. Mp 2190°. Bp 3660°. At high temp. reacts with all non-metals except H, Ge, Te and noble gases. Reacts with F_2 at r.t., H_2O at 100° → H_3BO_3. Non-toxic.

▷ ED7350000.

α-Rhombohedral-form

Consists of B_{12} icosahedra, with sl. deformed cep. 12 B atoms per unit cell. Synth. at 800-1100°. Obt. by pyrolysis of BI_3 on Ta, W or BN surface; also by pyrolysis of B hydrides. Cryst. from B-Pt melts. d 2.46.

α-Tetragonal-form

α′-form

1st cryst. polmorph obt. (1943). Now thought to be $B_{50}C_2$ or $B_{50}N_2$. There are 50 B atoms per unit cell with layers of B_{12} icosahedra connected by single B atoms. From $BBr_3 + H_2$ over Ta or W at 1200-1400°. d 2.35.

β-Rhombohedral-form

Thermodynamically most stable form. Struct. comprises central B_{12} icosahedron surrounded by an icosahedron of icosahedra. B-B 162-172, 176-177 and 188-192 pm. 105 atoms per unit cell. Synth. by cryst. of fused B. Mp 2250° (2180°), ~3650°. d 2.35.

β-Tetragonal-form

β′-form

192 B atoms per unit cell.

[14798-12-0, 14798-13-1]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1923, **5**, 1; *Suppl.* A, 1980; *Suppl.* B1, 1981 (*rev, bibl*)

Gmelin Handbook Inorg. Chem., Syst. No. 13, 1926; *Suppl.*, 1954 (*rev, bibl*)

Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 665.

Greenwood, N.N., *Boron*, Pergamon, Oxford, 1975.

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 787 (*synth*)

Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977.

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 62 (*rev, bibl*)

Kelly, R.G., *NMR Newly Accessible Nuclei*, (Ed. Laszlo, P.), Academic Press, N.Y., 1983, **2**, 49 (*B-11 nmr*)

Yakel, H.L. *et al*, *Am. Inst. Phys. Conf. Proc.*, 1986, **140**, 97 (*struct, rev*)

Shelnutt, J.A. *et al*, *Am. Inst. Phys. Conf. Proc.*, 1986, **140**, 312 (*α-form, raman*)

Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 155 (*rev*)

Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 34.

Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 745 (*tox*)

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 56 (*haz*)

IC-000765

[BBa]

Barium borides

[97793-30-1]

In addition to the hexaboride, the diboride has been reported, but its existence is in some doubt.

***Barium boride* (BaB_6), 9Cl, 8Cl** [12046-08-1]

Barium hexaboride

B_6Ba M 202.1

Possesses the CaB_6 struct. Synth. from Ba and B under H_2 at 800-1300°; $BaCl_2$ with $Ba_2B_2O_5$; $BaO + B_4C + B$ at 1500°. Good cathode material. Forms dark green cube-shaped single cryst. Mp ca. 2270°. Semiconductor.

Peshev, P., *Rev. Int. Hautes Temp. Refract.*, 1967, **4**, 299 (*synth*)

Markovskii, L.Ya. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1824; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1752 (*synth*)

Serebryakova, T.I. *et al., Poroshk. Metall. (Kiev).* 1969, **9**, 4; *Soc. Powder Metall. Met. Ceram. (Engl. Transl.).* 1969, **9**, 508 (*synth*)
Tsirkat, K. *et al., Mikrochk. Chem.*, 1971, **102**, 249; 1972, **103**, 744 (*cmbh*)
Matsuoka, S. *et al., J. Crystal Growth*, 1974, **26**, 165 (*synth, single cryst*)
Ishii, M. *et al., Solid State Commun.*, 1976, **20**, 437 (*synth, raman*)
Boron and Refractory Borides (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Aida, T. *et al., J. Appl. Phys.*, 1981, **52**, 1022 (*synth, props*)
Sears, R.E.J., *J. Chem. Phys.*, 1982, **76**, 5651 (*B-11 nmr*)

IC-000766

[BBe]

Beryllium borides

[66103-46-6]

Several phases reported; the existence of some is in doubt.

***Beryllium boride (Be$_3$B)*, 9CI, 8CI** [12536-51-5]

BBe_3 M 55.8

Mp 1160°. Fairly reactive to O, N, and C.

***Beryllium boride (Be$_2$B)*, 9CI, 8CI** [12536-51-5]

BBe_2 M 28.8

Fluorite struct. Synth. from B + Be at 1000°. Exists in pink and salmon-red forms.

***Beryllium boride (BeB$_2$)*, 9CI, 8CI** [12228-40-9]

B_2Be M 30.6

AlB_2-type struct. with hexagonal lattice. Synth. from elements at 800-1500° in inert atm. Potentially useful ceramic. Mp > 1970°. Stable to 800-900°.

***Beryllium boride (BeB$_6$)*, 9CI, 8CI** [12429-94-6]

Beryllium hexaboride

B_6Be M 73.8

Tetragonal lattice. B atoms occupy pairs of gaps in the packing of B_{12} icosahedra. Synth. from Be and B at 1000° (1400-1600°). Potential ceramic material and constituent of lightweight armour. Brick-red solid. Stable to 800-900°.

Sands, D.E. *et al., Acta Crystallogr.*, 1961, **14**, 309 (*synth, cryst struct*)
Hoenig, C.L. *et al., J. Am. Ceram. Soc.*, 1961, **44**, 385 (*synth, props*)
Matkovich, V. *et al., Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1965, **112**, 116 (*struct*)
Neshpor, V.S. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 10; *Inorg. Materials (Engl. Transl.)*, 1971, **7**, 45 (*rev*)
Tupitsyn, I.I. *et al., Fiz. Tverd. Tela (Leningrad)*, 1974, **16**, 3117; *Soviet Physics Solid State*, 1974, **16**, 2015 (*pe*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

HBe_2HO_4 **IC-000767**

Beryllium borate hydroxide ($Be_2(BO_3)(OH)$)

[1318-62-3]

$Be_2(OH)(BO_3)$ or $3BeO.Be(OH)_3.B_2O_3$

M 93.8

Contains planar $BO_3^{3\ominus}$ and $OH^{\ominus}$ ions, not tetrahedral $(BO_3OH)^{4\ominus}$ ions. Colourless or pale grey orthorhombic luminescent cryst.

☢ Highly toxic.

Mineral-form

Hambergite

Occasionally contains fluorine: $Be_2BO_3(OH,F)$. Found in Norway, Madagascar, India, Pakistan and USA. Colourless, white prismatic cryst.

Debruyn, C., *Proc. Int. Meeting Mod. Spectrosc., 4th, Bologna*, 1959, **2**, 717; *C.A.* 1963, **59**, 14715h (*ir*)
Zachariasen, W.H. *et al., Acta Crystallogr.*, 1963, **16**, 1144 (*cryst struct*)

Gerard, W.C.S. *et al., Compt. Rend. Hebd. Seances Acad. Sci.*, 1964, **259**, 337 (*raman*)
Switzer, G. *et al., Am. Mineral.*, 1965, **50**, 85 (*mineral*)

IC-000768

BBrClF

Bromochlorofluoroborane, 11Cl, 9Cl

Boron bromide chloride fluoride, 8Cl

[14720-22-0]

BBrClF

M 145.1

Formed in mixt. of BBr_3, BCl_3 and BF_3.

Coyle, T.D. *et al., J. Chem. Phys.*, 1960, **32**, 1892 (*synth, F-19 nmr*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Fieldhouse, S.A. *et al., J. Phys. Chem.*, 1969, **73**, 275 (*F-19 nmr*)
Pedley, J.B. *et al., J. Chem. Soc. A*, 1971, 2426 (*B-11 nmr*)

IC-000769

BBrClI

Bromochloroiodoborane, 11Cl, 9Cl

Boron bromide chloride iodide, 8Cl

[13709-69-8]

BBrClI

M 253.0

Formed in mixts. of BBr_3, BCl_3 and BI_3.

Delwaulle, M.L. *et al., Bull. Soc. Chim. Fr.*, 1957, 1101 (*synth, raman*)
Gates, P.N. *et al., J. Chem. Soc.*, 1964, 3511 (*synth, B-11 nmr*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Cerf, C., *Bull. Soc. Chim. Fr.*, 1971, 415 (*raman*)

$BBrCl_2$ **IC-000770**

Bromodichloroborane, 11Cl, 10Cl, 9Cl

Boron bromide chloride, 8Cl

[13709-70-1]

$BBrCl_2$

M 161.6

Formed in mixts. of BBr_3 and BCl_3. Sol. CH_2Cl_2; mod. sol. methylcyclohexane.

Gates, P.N. *et al., J. Chem. Soc.*, 1964, 3511 (*synth, B-11 nmr*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Wolfe, D.F. *et al., J. Mol. Struct.*, 1969, **3**, 293 (*ir*)
Cerf, C., *Bull. Soc. Chim. Fr.*, 1971, 415 (*raman*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1971, 383 (*synth, B-11 nmr*)

BBrFI **IC-000771**

Bromofluoroiodoborane, 11Cl, 9Cl

Boron bromide fluoride iodide, 8Cl

[22268-28-6]

BBrFI

M 236.6

Formed in mixts. of BBr_3, BF_3 and BI_3.

Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Pedley, J.B. *et al., J. Chem. Soc. A*, 1971, 2426 (*synth, B-11 nmr*)

$BBrF_2$ **IC-000772**

Bromodifluoroborane, 11Cl, 10Cl, 9Cl

Boron bromide fluoride, 8Cl

[14720-23-1]

$BBrF_2$

M 128.7

Formed in mixts. of BBr_3 and BF_3. Sol. CH_2Cl_2; mod. sol. methylcyclohexane.

Linderman, L.P. *et al., J. Phys. Chem.*, 1956, **24**, 242 (*synth, ir, raman*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Wolfe, D.F. *et al., J. Mol. Struct.*, 1969, **3**, 293 (*ir*)
Fieldhouse, S.A. *et al., J. Phys. Chem.*, 1969, **73**, 275 (*F-19 nmr*)
Pedley, J.B. *et al., J. Chem. Soc. A*, 1971, 2426 (*B-11 nmr*)

IC-000773

$BBrI_2$

Bromodiiodoborane, 11Cl, 9Cl

Boron bromide iodide, 8Cl

[14355-21-6]

$BBrI_2$

M 344.5

Formed in mixts. of BBr_3 and BI_3. Sol. CH_2Cl_2; mod. sol. methylcyclohexane.

Gates, P.N. *et al., J. Chem. Soc.*, 1964, 3511 (*synth, B-11 nmr*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Wolfe, D.F. *et al., J. Mol. Struct.*, 1969, **3**, 293 (*ir*)
Cerf, C., *Bull. Soc. Chim. Fr.*, 1971, 415 (*raman*)
Pedley, J.B. *et al., J. Chem. Soc. A*, 1971, 2426 (*synth, B-11 nmr*)

IC-000774

BBrO

Bromooxoborane, 11Cl, 9Cl

Boron bromide oxide. Boron oxybromide

[38490-24-3]

BOBr

M 106.7

Obt. as matrix isol. species at low temps.

Snelson, A., *High Temp. Sci.*, 1972, **4**, 318 (*synth, ir*)

BBr_2Cl **IC-000775**

Dibromochloroborane, 11Cl, 10Cl, 9Cl

Boron bromide chloride, 8Cl

[13709-71-2]

BBr_2Cl

M 206.0

Formed in mixts. of BBr_3 and BCl_3. Sol. CH_2Cl_2, mod. sol. methylcyclohexane.

Gates, P.N. *et al., J. Chem. Soc.*, 1964, 3511 (*synth, B-11 nmr*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105; 1971, 383 (*synth, ms, B-11 nmr*)
Wolfe, D.F. *et al., J. Mol. Struct.*, 1969, **3**, 293 (*ir*)
Cerf, C., *Bull. Soc. Chim. Fr.*, 1971, 415 (*raman*)

BBr_2F **IC-000776**

Dibromofluoroborane, 11Cl, 10Cl, 9Cl

Boron bromide fluoride, 8Cl

[14720-25-3]

BBr_2F

M 189.6

Formed in mixts. of BBr_3 and BF_3. Sol. CH_2Cl_2; mod. sol. methylcyclohexane.

Linderman, L.P. *et al., J. Phys. Chem.*, 1956, **24**, 242 (*synth, ir, raman*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Wolfe, D.F. *et al., J. Mol. Struct.*, 1969, **3**, 293 (*ir*)
Fieldhouse, S.A. *et al., J. Phys. Chem.*, 1969, **73**, 275 (*F-19 nmr*)
Pedley, J.B. *et al., J. Chem. Soc. A*, 1971, 2426 (*B-11 nmr*)

BBr_2H **IC-000777**

Dibromoborane, 10Cl, 9Cl, 8Cl

Dibromoborine

[13709-65-4]

BBr_2H

M 171.6

Prototype of the series of alkyldibromoboranes. Readily disproportionates into diborane, monobromoborane and BBr_3. More stable as its dimethyl sulfide complex. Unstable gas, sensitive to moisture. Reacts with hydroxylic solvs. and more slowly with ethers.

Me_2S complex: [55671-55-1]. *Dibromo(dimethyl sulfide) hydroboron. Dibromohydro[thiobis[methane]]boron, 10Cl*

$C_2H_7BBr_2S$ M 233.7

Hydroborating agent for alkenes and alkynes with high regiospecificity; provides a route to alkyldibromoboranes and alkyldihydroxyboranes. Air- and moisture-sensitive solid. Mp 30-33°.

Et_2O complex: [71648-08-3]. *Dibromo(diethyl ether) hydroboron. Dibromohydro[1,1'-oxybis[ethane]]boron, 10Cl. Dibromoborane etherate*

$C_4H_{11}BBr_2O$ M 245.7

Moisture-sensitive. Characterised only by ^{11}B nmr.

Dimer: Tetrabromodiborane(5)

$B_2Br_4H_2$ M 343.2

Existence not confirmed.

U.K. Pat., 853 379, (1960); *C.A.* **55**, 18553d (*synth*)
Rietti, S.B. *et al., J. Inorg. Nucl. Chem.*, 1965, **27**, 247 (*synth, ir*)
Lynds, L., *Spectrochim. Acta*, 1966, **22**, 2123 (*ir*)
U.S. Pat., 3 323 867, (1967); *C.A.* **67**, 55772s (*synth*)
Bouix, J. *et al., Bull. Soc. Chim. Fr.*, 1968, 3157 (*synth, props*)
Brown, H.C. *et al., Inorg. Chem.*, 1977, **16**, 2938 (*deriv, synth, nmr*)
Brown, H.C. *et al., J. Am. Chem. Soc.*, 1977, **99**, 7097
Hu, M.G. *et al., Inorg. Chem.*, 1979, **18**, 3297 (*deriv, synth, nmr*)
Brown, H.C. *et al., J. Org. Chem.*, 1980, **45**, 384, 389 (*deriv, usr*)
Frost, D.C. *et al., J. Am. Chem. Soc.*, 1981, **103**, 4428 (*synth, pe*)

BBr_2I **IC-000778**

Dibromoiodoborane, 11Cl, 10Cl, 9Cl

Boron bromide iodide, 8Cl

[13709-72-3]

BBr_2I

M 297.5

Formed in mixts. of BBr_3 and BI_3. Sol. CH_2Cl_2; mod. sol. methylcyclohexane.

Gates, P.N. *et al., J. Chem. Soc.*, 1964, 3511 (*synth, B-11 nmr*)
Lappert, M.F. *et al., J. Chem. Soc. A*, 1968, 3105 (*synth, ms*)
Wolfe, D.F. *et al., J. Mol. Struct.*, 1969, **3**, 293 (*ir*)
Cerf, C., *Bull. Soc. Chim. Fr.*, 1971, 415 (*raman*)
Pedley, J.B. *et al., J. Chem. Soc. A*, 1971, 2426 (*synth, B-11 nmr*)

BBr_3 **IC-000779**

Tribromoborane, 11Cl, 10Cl, 9Cl

Boron tribromide. Boron bromide (BBr_3), 9CI

[10294-33-4]

BBr_3

M 250.5

Commercially available. Reagent for preparation of other B compds. Catalyst in polym., alkylation and acylation reactions. Ultra-pure material used to produce B-doped semiconductors. Colourless liq., v. moisture sensitive. Sol. CCl_4, SO_2 (l), SCl_2; mod. sol. methylcyclohexane. Mp −46° Bp 91.3° ΔH_f −208 kJ mol^{-1}; ΔH_{vap} −35 kJ mol^{-1}.

▷ Corrosive. Reacts violently with H_2O. ED7400000.

Skinner, H.A. *et al, Trans. Faraday Soc.*, 1955, **51**, 19 (*thermochem*)
Koski, W.S. *et al, J. Am. Chem. Soc.*, 1959, **81**, 1326 (*ms*)
Laurita, W.G. *et al, J. Am. Chem. Soc.*, 1959, **81**, 3179 (*nqr*)
Konaka, S. *et al, Bull. Chem. Soc. Jpn.*, 1966, **39**, 1146 (*ed*)
Nöth, H. *et al, Chem. Ber.*, 1966, **99**, 1049 (*B-11 nmr*)
Shimanouchi, T., *J. Phys. Chem. Ref. Data*, 1977, **6**, 993 (*ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, Suppl. Vol., 1978, **53**, 1 (*rev, usex*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 129 (*usex, haz*)

BBr_3Cl_3P IC-000780

Trichloro(phosphorous tribromide)boron
Trichloroborane phosphorus tribromide. Boron trichloride-phosphorus tribromide adduct
[85745-60-4]

$Cl_3B\text{-}PBr_3$

M 387.8
Unstable at −40°.
Arnington, A.F. *et al, Inorg. Chem.*, 1966, **5**, 483 (*synth*)

BBr_3H_3P IC-000781

Tribromo(phosphine)boron
Boron tribromide-phosphine adduct. Tribromoborane-phosphine compd. (1:1), 9CI
[38622-66-1]

$Br_3B\text{-}PH_3$

M 184.5
Colourless solid. Spar. sol. MeI; sol. CH_2Cl_2.
Drake, J.E. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2341; 1974, 923 (*synth, pmr, ir, raman*)
Durig, J.R. *et al, Inorg. Chem.*, 1974, **13**, 2729 (*ir, raman*)
Drake, J.E. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 2613 (*B-11 nmr, ir, raman*)

$BBr_4^\ominus$ IC-000782

Tetrabromoborate(1 −), 11Cl, 10Cl, 9Cl, 8Cl
[14911-68-3]

$[BBr_4]^\ominus$ (T_d)

M 330.4 (ion)
NH_4 salt: Ammonium tetrabromoborate
BBr_4H_4N M 348.4
V. hygroscopic colourless cryst. Sol. HBr; $PhNO_2$; mod. sol. CH_2Cl_2.
Et_4N salt: [23391-70-0].
V. hygroscopic colourless cryst. (CH_2Cl_2.) Sol. MeCN. Insol. C_6H_6, CCl_4, Et_2O, pentane, CS_2. Mp 278-280°.
Pyridinium salt: V. hygroscopic, colourless cryst. Mod. sol. CH_2Cl_2. Insol. C_6H_6, Et_2O, CCl_4, CS_2, pentane. Mp 140-142° dec.

Lappert, M.F., *Proc. Chem. Soc., London*, 1957, 121 (*synth*)
Kynaston, W. *et al, J. Chem. Soc.*, 1960, 1772 (*synth, ir*)
Thompson, R.J. *et al, Inorg. Chem.*, 1965, **4**, 1464 (*B-11 nmr*)
Creighton, J.A., *J. Chem. Soc.*, 1965, 6389 (*ir*)
Beecher, J.M. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 823 (*synth*)
Ahmad, I.Y. *et al, Inorg. Chem.*, 1969, **8**, 1411 (*synth, ir, conductance*)
Shirai, S.U., *Bull. Chem. Soc. Jpn.*, 1970, **43**, 2879 (*synth, thermal anal*)
Harris, R.K. *et al, Spectrochim. Acta, Part A*, 1983, **39**, 309 (*solid state B-11 nmr*)

BBr_6P IC-000783

Tribromo(phosphorous tribromide)boron
Boron tribromide-phosphorus tribromide adduct. Tribromoborane phosphorous tribromide. Boron bromide-phosphorus bromide compd. (1:1), 8CI
[15194-82-8]

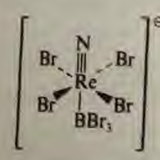
Br_3BPBr_3

M 521.2
Colourless solid, stable *in vacuo*. Rel. insol. CS_2. Mp 61-62°. ΔH_f −178.4 kJ mol^{-1}.

Tarible, J., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1893, **116**, 1521 (*synth*)
Holmes, R.R., *J. Inorg. Nucl. Chem.*, 1960, **12**, 266 (*synth*)
Arnington, A.F. *et al, Inorg. Chem.*, 1966, **5**, 483 (*synth*)
Finch, A. *et al, Inorg. Chem.*, 1967, **6**, 386 (*thermochem*)
Terao, H. *et al, Bull. Chem. Soc. Jpn.*, 1983, **56**, 1728 (*nqr*)

$BBr_7NRe^\ominus$ IC-000784

(Boron tribromide)tetrabromonitridorhenate(*VI*)(1 −)
[Aminotribromoborato(3 −)]tetrabromorhenate(VI)(1 −), 11Cl (incorr.)



M 770.3 (ion)
Believed distorted octahedral as shown with BBr_3 occupying sixth position. Ir $\nu_{Re\equiv N}$ 1170 cm^{-1}. See also Tetrabromonitridorhenate(*VI*)(1 −), IC-002043.
Ph_4As salt: [83678-71-1].
Synth. from $AsPh_4[ReNCl_4]$ and BBr_3 at 90°. Deep violet powder. Sol. CH_2Br_2.
▷ Fumes in air.

Kaftz, W. *et al, Z. Anorg. Allg. Chem.*, 1982, **490**, 175 (*synth, ir, prepn*)

[BCa] IC-000785

Calcium borides
[39377-46-3]

Calcium boride* (CaB_2), *9CI, 8CI [103981-17-5]
Calcium diboride
B_2Ca M 61.7

Calcium boride* (CaB_6), *9CI, 8CI [12007-99-7]
Calcium hexaboride
B_6Ca M 104.9
Cubic lattice with Ca at cell centre and compact, regular octahedra of B atoms linked at vertices by B—B bonds to give 3-D B network. Synth. from B_4C or B with Ca or CaO at 800-1600°; or from CaO + H_3BO_3 + Mg at 1100°. Also from $CaCO_3$ + B. Used in the manuf. of boron-alloyed steel. Black prisms or platelets. Insol. H_2O, MeOH. EtOH. Dissolves slowly in acids. Mp 2235°. Dec. to Ca + B in vapour. Semiconductor.

Blum, H. *et al, Acta Crystallogr.*, 1954, **7**, 81 (*struct, CaB_6*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 804 (*rev, bibl*)
Tonkina, V.V. *et al, Zh. Prikl. Khim. (Leningrad)*, 1966, **39**, 1468; *J. Appl. Chem. USSR (Engl. Transl.)*, 1966, **39**, 1375 (*synth, ms*)
Petzlow, P., *Rev. Int. Hautes Temp. Refract.*, 1967, **4**, 289 (*synth*)
Markovskii, L.Ya. *et al, Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1824; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1752 (*synth*)
Niemyski, T. *et al, J. Less-Common Met.*, 1968, **15**, 97 (*purif*)

Serebryakova, T.I. *et al, Poroshk. Metall. (Kiev)*, 1969, **9**, 4; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, **9**, 608 (*synth*)
Rea, J.R. *et al, J. Crystal Growth*, 1971, **11**, 110 (*synth*)
Muranaka, S. *et al, J. Crystal Growth*, 1974, **26**, 165 (*synth, single cryst, struct*)
Ishii, M. *et al, Solid State Commun.*, 1976, **20**, 437 (*synth, raman*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, 1977 (*rev, bibl*)
Perkins, P.E., *Boron Refract. Borides*, 1977, 31; *CA*, 1978, **88**, 55228 (*electronic struct*)
Ihara, H., *CA*, 1978, **89**, 155195 (*pe, theory*)
Aleshin, V.G. *et al, J. Less-Common Met.*, 1979, **67**, 173 (*pe*)
Aono, M. *et al, J. Phys. Chem. Solids*, 1979, **40**, 797 (*synth, B-11 nqr*)
Sears, R.E., *J. Chem. Phys.*, 1982, **76**, 5651 (*B-11 nmr*)
Hauffe, K., *Z. Werkstoffled*, 1984, **13**, 427; *CA*, 1985, **207**, 99265 (*corrosion resistance, F_2, HF*)

$BCaHO_3Si$ IC-000786

Datolite, 9CI
[1318-40-7]

$HCa[BSiO_5]$

M 159.9
Mineral. A single layer silicate. Occurs as a secondary mineral in basic igneous rocks. A minor gem material. Colourless monoclinic prismatic cryst. tinted greenish, pink, reddish, or brownish by impurities.

Deer, W.A. *et al, Rock Forming Minerals*, Longman, London, 1962, **1**, 171 (*rev*)
King, G.S.D. *et al, Bull. Mineral.*, 1988, **111**, 431 (*rev*)
Foit, F.F. *et al, Am. Mineral.*, 1973, **58**, 909 (*cryst struct*)
Speer, J.A. *et al, Rev. Mineral.*, 1982, **5**, 391 (*rev*)

[BCe] IC-000787

Cerium borides
[97793-35-6]

Cerium boride* (CeB), *9CI, 8CI [12045-00-0]
Cerium monoboride
BCe M 150.9
Existence not confirmed.

Cerium boride* (CeB_4), *9CI, 8CI [12007-52-2]
Cerium tetraboride
B_4Ce M 183.3
Tetragonal UB_4-type struct. Bronze-coloured plates. Mp 2380°, 2350° dec. Dec. at 2200° → CeB_6. Can be subl. in high vacuum without dec. Evidence for oxid. state near $Ce^{4\oplus}$ - exhibits temp. independent paramagnetism at 50-300K.

Cerium boride* (CeB_6), *9CI, 8CI [12008-02-5]
Cerium hexaboride
B_6Ce M 204.9
Has the CaB_6-type struct. Synth. by electrolysis of $CeCl_3$ in KBF_4 with B_4C anode; or from CeO_2 + H_3BO_3 + Mg at 1300°. Bluish cryst. Mp 2190°. Fairly stable to HCl, dil. H_2SO_4 but dissolves easily in HNO_3 or conc. H_2SO_4 with dec. Subl. without dec. in high vacuum. At 1400-1900° → 'CeB'. Metallic conductor. μ_{eff} = 2.49μ_B.

Zalkin, A. *et al, Acta Crystallogr.*, 1953, **6**, 269 (*cryst struct*)
Tonkina, V.V. *et al, Zh. Prikl. Khim. (Leningrad)*, 1966, **39**, 1468; *J. Appl. Chem. USSR (Engl. Transl.)*, 1966, **39**, 1375 (*synth, ms*)
Paderno, Yu.B. *et al, Phys. Status Solidi*, 1967, **24**, K73 (*magnetism, CeB_6*)
Niemyski, T. *et al, J. Less-Common Met.*, 1968, **15**, 97 (*purif*)
Nanneveta, M. *et al, Rev. Int. Hautes Temp. Refract.*, 1968, **5**, 229 (*synth*)
Brückow, K.H.J. *et al, J. Chem. Phys.*, 1972, **57**, 3910 (*magnetism*)
Fisk, Z. *et al, Mater. Res. Bull.*, 1972, **7**, 285 (*synth, single cryst, cryst struct*)
Amici, L.L. *et al, High Temp. Sci.*, 1975, **7**, 44 (*ms*)

Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Etourneau, J. *et al, J. Chem. Phys.*, 1979, **67**, 531 (*synth, CeB_4*)
Sobczak, R.J. *et al, J. Less-Common Met.*, 1979, **67**, 167 (*synth, CeB_6*)
Tanaka, T. *et al, J. Appl. Phys.*, 1980, **51**, 3877 (*synth, purif*)
Kawakimi, M. *et al, J. Phys. Soc. Jpn.*, 1981, **50**, 432 (*B-11 nmr*)
Sugawara, H. *et al, J. Phys. Soc. Jpn.*, 1982, **51**, 915 (*pe*)
Zir ngriebl, E. *et al, Phys. Rev. B*, 1984, **30**, 4052 (*raman*)
Eliseev, A.A. *et al, Kristallografiya*, 1986, **31**, 803 (*cryst struct, CeB_6*)
Kasuya, T. *et al, J. Magn. Magn. Mater.*, 1988, **76/77**, 46 (*cryst field spectrosc, CeB_6*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1990, **C11a**, 6, 21 (*rev*)

BCe_2Fe_{14} IC-000788

Cerium iron boride ($Ce_2Fe_{14}B$)
[93388-48-8]

$Ce_2Fe_{14}B$

M 1072.8
Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. Magnetic recording material. T_c 431K. Absorbs hydrogen.

Andreev, A.V. *et al, Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)
Pinkerton, F.E. *et al, J. Appl. Phys.*, 1985, **57**, 4121 (*mössbauer, struct*)
Dub, O.M. *et al, CA*, 1986, **105**, 201912 (*synth, cryst struct*)
Rosenberg, M. *et al, Hyperfine Interact.*, 1986, **28**, 503 (*mössbauer, struct*)
Herbst, J.F. *et al, J. Magn. Magn. Mater.*, 1986, **54-57**, 570 (*cryst struct*)

$BClF_2$ IC-000789

Chlorodifluoroborane
Boron chloride fluoride
[14720-30-0]

BF_2Cl

M 84.2
Moisture-sensitive gas. ΔH_f° −886 kJ mol^{-1}.
Et_3N complex: [82862-09-7].
$C_6H_{15}BClF_2N$ M 185.4
^{19}F nmr δ −127.8 (J_{BF} 46.9 Hz) ppm.
N-Ethylaniline complex: [82862-91-7].
$C_8H_{11}BClF_2N$ M 205.4
^{19}F nmr δ −132.8 (J_{BF} 40.7 Hz) ppm.
N-Ethyl-N-methylaniline complex: [82862-48-4].
$C_9H_{13}BClF_2N$ M 219.4
^{19}F nmr δ −136.5;^{11}B nmr δ 4.3 (J_{BF} 43.1 Hz) ppm.

Porter, R.F. *et al, J. Chem. Phys.*, 1962, **36**, 2104 (*synth*)
Fox, A. *et al, J. Heterocycl. Chem.*, 1982, 1275 (*deriv, F-19 nmr, B-11 nmr, cmr*)

$BClF_3^\ominus$ IC-000790

Chlorotrifluoroborate(1 −), 11Cl, 10Cl, 9Cl, 8Cl
[36503-32-9]

$[BClF_3]^\ominus$

M 103.2 (ion)
Me_4N salt: Colourless solid. Sol. CH_2Cl_2.
Tetrachlorophosphonium salt:
BCl_5F_3P M 276.0
Colourless solid. Sol. anhyd. HCl.

Waddington, T.C. *et al, J. Chem. Soc.*, 1960, 2332, 2339 (*synth, ir*)

Wharf, I. et al, J. Inorg. Nucl. Chem., 1970, 32, 183 (synth, ir)
Hartman, J.S. et al, Inorg. Chem., 1972, 11, 940 (B-11 nmr, F-19 nmr)
Hunt, R.L. et al, Spectrochim. Acta, Part A, 1981, 37, 63 (ir)

IC-000791

$BClH_2$

Chloroborane, 10Cl, 9Cl

Chloroborane

[10388-28-0]

$BClH_2$

M 48.2

Prototype of the dialkylchloroboranes. Prepd. from diborane and boron trichloride. Early reports of synth. in THF may be unreliable. Stability better in Et_2O. Hydroborating reagent (in Et_2O). Relatively stable in prod. equilibrium mixt., but probably as Et_2O complex. Sol. Et_2O

Et_2O adduct: [36594-41-9]. *Chloro(diethyl ether)dihydroboron. Chlorodihydro[1,1'-oxybis[ethane]]boron, 10Cl. Chloroborane compd. with 1,1'-oxybis[ethane] (1:1), 9Cl. Monochloroborane diethyl etherate*

$C_4H_{12}BClO$ M 122.4

Used in prepn. of dialkylchloroboranes by hydroboration of alkenes. Stable at 0° for several weeks (under N_2); moisture-sensitive.

Schlesinger, H.I. et al, J. Am. Chem. Soc., 1931, 53, 4321 (synth)
Kerrigan, J.V., Inorg. Chem., 1964, 3, 908 (synth, ir)
Zweifel, G., J. Organomet. Chem., 1967, 9, 215 (synth, props)
Pasto, D.J. et al, J. Am. Chem. Soc., 1968, 90, 3797 (props, synth)
Brown, H.C. et al, J. Am. Chem. Soc., 1972, 94, 2112 (deriv, synth)
Carlson, B.A. et al, J. Am. Chem. Soc., 1973, 95, 6876 (deriv)
Brown, H.C. et al, J. Org. Chem., 1973, 38, 182; 1976, 98, 1785; 1979, 44, 2422 (deriv)
Yamamoto, Y. et al, Yuki Gosei Kagaku Kyokaishi, 1974, 32, 544 (rev)
Hu, M.G. et al, Inorg. Chem., 1979, 18, 3297 (deriv, nmr)
Kagoyuk, D.S. et al, Zh. Fiz. Khim., 1980, 54, 60
Arase, A. et al, Bull. Chem. Soc. Jpn., 1981, 54, 299

IC-000792

$BClH_3^{\ominus}$

Chlorotrihydroborate(1−), 11Cl, 10Cl

Chlorohydroborohydride

[68011-52-9]

$[BClH_3]^{\ominus}$ (C_{3v})

M 49.2 (ion)

Tetrabutylammonium salt: [69969-99-9]. Colourless solid. Sol. CH_2Cl_2.

Taft, M.A. et al, Inorg. Chem., 1982, 21, 1952 (synth, ir, B-11 nmr)
Lawrence, S.H., Diss. Abstr. Int., B, 1984, 45, 1773 (synth, ir, B-11 nmr, pmr)

IC-000793

$BClI_2$

Chlorodiiodoborane, 11Cl, 9Cl

Boron chloride iodide, 8Cl

[13709-74-5]

$BClI_2$

M 300.0

Formed in mixts. of BCl_3 and BI_3. Sol. CH_2Cl_2; mod. sol. methylcyclohexane.

Gates, P.N. et al, J. Chem. Soc., 1964, 3511 (synth, B-11 nmr)
Lappert, M.F. et al, J. Chem. Soc. A, 1968, 3105 (synth, ms)
Wolfe, D.F. et al, J. Mol. Struct., 1969, 3, 293 (ir)
Cerf, C., Bull. Soc. Chim. Fr., 1971, 415 (raman)
Pedley, J.B. et al, J. Chem. Soc. A, 1971, 2426 (B-11 nmr)

IC-000794

BClO

Chlorooxoborane, 11Cl, 9Cl

Boron chloride oxide, 8Cl. Boron oxychloride

[23361-55-9]

BClO

M 62.2

Unstable molecule. Synth. in gas phase by electric discharge through BCl_3/O_2 mixt.

Snelson, A., High Temp. Sci., 1972, 4, 318 (ir)
Kawaguchi, K. et al, J. Mol. Spectrosc., 1982, 93, 381 (synth, microwave)

IC-000795

BClS

Chlorothioxoborane, 11Cl, 10Cl

Boron chloride sulfide

[55753-38-3]

BClS

M 78.3

Unstable gas phase molecule. Synth. at 800-1000°.

Blauer, J. et al, Trans. Faraday Soc., 1964, 60, 301 (synth, ms)
Snelson, A., High Temp. Sci., 1972, 4, 318 (ir)
Kirby, C. et al, J. Am. Chem. Soc., 1978, 100, 3766 (synth, microwave, pe)
Kirby, C. et al, J. Mol. Spectrosc., 1980, 83, 130 (microwave)

IC-000796

BCl_2F

Dichlorofluoroborane, 11Cl, 10Cl, 9Cl

Boron chloride fluoride, 8Cl

[14720-31-1]

BCl_2F

M 100.7

Formed in mixts. of BCl_3 and BF_3.

Lappert, M.F. et al, J. Chem. Soc. A, 1968, 3105 (synth, ms)
Wolfe, D.F. et al, J. Mol. Struct., 1969, 3, 293 (ir)
Fieldhouse, S.A. et al, J. Phys. Chem., 1969, 73, 275 (F-19 nmr)
Pedley, J.B. et al, J. Chem. Soc. A, 1971, 2426 (B-11 nmr)
Kroto, H.W. et al, J. Chem. Soc., Chem. Commun., 1975, 810 (microwave, pe)
Kroto, H.W. et al, J. Mol. Spectrosc., 1977, 65, 280 (microwave)

IC-000797

BCl_2H

Dichloroborane, 10Cl, 9Cl

Dichloroborine

[10325-39-0]

BCl_2H

M 82.7

Prototype of series of alkyldichloroboranes; often formed with chloroborane and trichloroborane, and not easily purified. Prob. dimeric in the free state. Useful hydroborating agent as its dimethyl sulfide or Et_2O complexes, though may require addition of BCl_3 in order to react. Gas, readily disproportionates; air- and moisture-sensitive. ΔH_f° −257 kJ mol^{-1}.

Me_2S adduct: [63462-42-0]. *Dichloro(dimethyl sulfide)hydroboron. Dichlorohydro[thiobis[methane]]boron, 10Cl*

$C_2H_7BCl_2S$ M 144.8

Stable hydroborating agent with high reaction regiospecificity. Clear viscous liq., remarkably stable although slow dec. by moisture.

Et_2O adduct: [41156-66-5]. *Dichloro(diethyl ether)hydroboron. Dichlorohydro[1,1'-oxybis[ethane]]boron, 10Cl. Dichloroborane [1,1'-oxybis(ethane)], 9Cl. Dichloroborane ethyl etherate, 8Cl*

$C_4H_{11}BCl_2O$ M 156.8

Reagent for general synth. of alkyl and alkenyl dichloroboranes via hydroboration. Air- and moisture-sensitive liq. Mp −27° to −23°.

Dimer: [94592-83-3]. *Tetrachlorodiborane(6), 11Cl*

$B_2Cl_4H_2$ M 165.4

Brown, H.C. et al, J. Inorg. Nucl. Chem., 1959, 9, 51 (deriv, synth)
U.K. Pat., 852 312, (1960); CA, 55, 23953c (synth)
Meyers, H.W. et al, Inorg. Chem., 1963, 2, 655 (synth, ir)
Lynds, L. et al, J. Chem. Phys., 1964, 40, 1590 (ir)
Zweifel, G. et al, J. Organomet. Chem., 1967, 9, 215 (synth)
Brown, H.C. et al, J. Am. Chem. Soc., 1973, 95, 2396; 1976, 98, 1798, 4917 (deriv, use)
Rockwood, S.D., Chem. Phys. Lett., 1975, 34, 542 (synth)
Brown, H.C. et al, J. Org. Chem., 1977, 42, 2533; 1980, 45, 384 (deriv, use)
Lin, C.T. et al, J. Chem. Phys., 1978, 68, 4233 (synth, ms)
Dodds, A.R. et al, Inorg. Chem., 1979, 18, 1465 (deriv, synth, nmr)
Frost, D.C. et al, J. Am. Chem. Soc., 1981, 103, 4428 (synth)

IC-000798

BCl_2HS

Dichloromercaptoborane, 11Cl, 10Cl

[39130-80-8]

$HSBCl_2$

M 114.7

Colourless liq. unstable above 0°.

Wartik, T. et al, J. Am. Chem. Soc., 1958, 80, 6155 (synth)
Bouix, J. et al, Can. J. Chem., 1973, 51, 292 (synth, ms, B-11 nmr)
Bouix, J. et al, J. Mol. Struct., 1973, 15, 103 (ir, raman)
Kirklin, D.R. et al, J. Mol. Spectrosc., 1977, 67, 322 (synth, ir, raman)

IC-000799

$BCl_2H_2^{\ominus}$

Dichlorodihydroborate(1−), 11Cl, 10Cl

Dichloroborohydride

[68011-51-8]

$[BCl_2H_2]^{\ominus}$

M 83.7 (ion)

Bis(triphenylphosphine)iminium salt: Colourless solid. Sol. CH_2Cl_2.

Lawrence, S.H., Diss. Abstr. Int., B, 1984, 45, 1773 (synth, ir, B-11 nmr, pmr)

IC-000800

BCl_2H_4LiMn

Lithium manganese borohydride chloride ($LiMn(BH_4)Cl_2$)

$LiMn(BH_4)Cl_2$

M 147.6

Struct. not known. Synth. from $LiBH_4$ and $MnCl_2$ in dry Et_2O.

Nöth, H., Angew. Chem., 1961, 73, 371 (synth)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, C7, 92 (rev, bibl)

IC-000801

BCl_2I

Dichlorolodoborane, 11Cl, 9Cl

Boron chloride iodide, 8Cl

[13709-76-7]

BCl_2I

M 208.6

Formed in mixts. of BCl_3 and BI_3. Sol. CH_2Cl_2; mod. sol. methylcyclohexane.

Gates, P.N. et al, J. Chem. Soc., 1964, 3511 (synth, B-11 nmr)
Lappert, M.F. et al, J. Chem. Soc. A, 1968, 3105 (synth, ms)
Wolfe, D.F. et al, J. Mol. Struct., 1969, 3, 293 (ir)
Cerf, C., Bull. Soc. Chim. Fr., 1971, 415 (raman)
Pedley, J.B. et al, J. Chem. Soc. A, 1971, 2426 (B-11 nmr)

IC-000802

BCl_3

Trichloroborane, 11Cl, 10Cl, 9Cl

Boron chloride (BCl_3), 8Cl. Boron trichloride

[10294-34-5]

BCl_3

M 117.1

Commercially available. Important starting material. Catalyst in polym. reactions, synth of halosilanes and in production of boron fibres. Colourless gas, v. easily hydrol. Sol. aprotic solvs. d_4^{11} 1.349. Mp −107°. Bp_{733} 12.5°. ΔH_f −289 kJ mol^{-1}, ΔH_{hyd} −403 kJ mol^{-1}.

▷ ED1925000.

Spencer, C. et al, J. Chem. Phys., 1958, 28, 355 (crystal struct at −163°)
Kanaka, S. et al, Bull. Chem. Soc. Jpn., 1966, 39, 1134 (ed)
Nöth, H. et al, Chem. Ber., 1966, 99, 1049 (B-11 nmr)
Dibeler, V.H. et al, Inorg. Chem., 1969, 8, 50 (ms)
Bassett, P.J. et al, J. Chem. Soc. A, 1971, 1551 (pe)
Planckaert, A.A. et al, Chem. Phys. Lett., 1973, 20, 170 (ur)
Shimanouchi, T., J. Phys. Chem. Ref. Data, 1977, 6, 993 (ir, raman)
Gmelin Handbook Inorg. Chem., Syst. No. 13, Suppl., 1978, 53 (rev, bibl)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 4, 129 (uses, haz)

IC-000803

$BCl_3F^{\ominus}$

Trichlorofluoroborate(1−), 11Cl, 10Cl, 9Cl

[36503-36-3]

$[BCl_3F]^{\ominus}$

M 136.1 (ion)

Tetrabutylammonium salt: Obt. in soln., not isol. Sol. CH_2Cl_2.

Hartman, J.S. et al, Inorg. Chem., 1972, 11, 940 (B-11 nmr, F-19 nmr)
Hunt, R.L. et al, Spectrochim. Acta, Part A, 1981, 37, 63 (ir)

IC-000804

BCl_3F_3P

Trichloro(phosphorous trifluoride)boron

Trichloroborane phosphorus trifluoride. Boron trichloride-phosphorus trifluoride adduct

[85745-57-9]

$Cl_3B\text{-}PF_3$

M 205.1

Compd. unknown, even at low temps.

Booth, H.S. et al, J. Am. Chem. Soc., 1943, 65, 2334 (attempted synth)
Massey, A.G., Adv. Inorg. Chem. Radiochem., 1967, 10, 54 (rev)

IC-000805

$BCl_3H^{\ominus}$

Trichlorohydroborate(1−), 10Cl

Trichloroborohydride

$[Cl_3BH]^{\ominus}$

M 118.1 (ion)
Tetrabutylammonium salt: [69969-98-8].
Selective reducing agent. Moisture-sensitive cryst. solid. Sol. THF, diglyme, arom. hydrocarbons; insol. alkanes.
▷ Dec. slowly at 110°, rapidly at 200°.

Titov, L.V. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1978, 1722; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1504 (*synth, ir, props*)
Kryshtal, G.V. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1981, 1146; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 907 (*use*)
Leach, J.B. *et al, J. Am. Chem. Soc.*, 1981, **103**, 988 (*synth, nmr*)

BCl_3H_3N IC-000806

Amminetrichloroboron
Trichloroborane ammonia; Boron trichloride-ammonia adduct
[49860-18-6]

$Cl_3B{\cdot}NH_3$

M 134.2
Minor product in reaction of H_3BNH_3 with BCl_3. Unstable with respect to elimination of HCl.

Hu, M.G. *et al, Inorg. Chem.*, 1979, **18**, 3297 (*synth*)
Hunt, R.L. *et al, Spectrosc. Int. J.*, 1982, **1**, 31 (*ir*)

BCl_3O_4 IC-000807

Dichloro(perchlorato)borane
Dichloro(perchloryloxy)borane, 10Cl
[15122-71-1]

Cl_2BOClO_3

M 181.1
Colourless liq. at −78°; glass at −180°.

Chausse, T. *et al, Nouv. J. Chim.*, 1981, **5**, 261 (*synth, ir, raman*)

BCl_3O_8 IC-000808

Chlorodiperchloratoborane
Chlorobis(perchloryloxy)borane, 10Cl
[15122-72-2]

$ClB(OClO_3)_2$

M 245.1
Colourless solid at −78°, dec. at r.t.

Chausse, T. *et al, Nouv. J. Chim.*, 1981, **5**, 261 (*synth, ir, raman*)

BCl_3O_{12} IC-000809

Triperchloratoborane
Boron triperchlorate; Boron perchlorate, 10Cl, 9Cl
[15122-73-3]

$B(OClO_3)_3$

M 309.1
Colourless cryst. solid at −78°, dec. slowly at r.t.
▷ Presumed explosive.

Mosher, R.A. *et al, CA*, 1966, **64**, 1598 (*synth*)
Chausse, T. *et al, Nouv. J. Chim.*, 1981, **5**, 261 (*synth, ir, raman*)

$BCl_4^{\ominus}$ IC-000810

Tetrachloroborate(1 −), 11Cl, 10Cl, 9Cl, 8Cl
[14911-67-2]

$[BCl_4]^{\ominus}$ (T_d)

M 152.6 (ion)
K salt: [31126-61-1]. *Potassium tetrachloroborate*
BCl_4K M 191.7
V. hygroscopic colourless solid. Sol. liq. SO_2.
Me_4N salt: [4272-49-5].
V. hygroscopic colourless solid. Sol. CH_2Cl_2. Insol. C_6H_6, CS_2, pentane, Et_2O. Mp 264° dec.
Pyridinium salt: V. hygroscopic colourless solid. Sol. MeCN. Insol. CCl_4, Et_2O, pentane, CS_2, C_6H_6. Mp 118-121° dec. (sealed tube).

Muetterties, E.L. *et al, J. Am. Chem. Soc.*, 1957, **79**, 6563 (*synth*)
Lappert, M.F., *Proc. Chem. Soc., London*, 1957, 121 (*synth*)
Kynaston, W. *et al, J. Chem. Soc.*, 1960, 1772 (*synth, ir*)
Thompson, R.J. *et al, Inorg. Chem.*, 1965, **4**, 1464 (*B-11 nmr*)
Creighton, J.A., *J. Chem. Soc.*, 1965, 6598 (*ir*)
Titova, K.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 597 (*synth*)
Drache, M., *Bull. Soc. Chim. Fr.*, 1976, 1749 (*synth*)
Sheikh, S.U., *J. Therm. Anal.*, 1980, **18**, 299 (*thermal anal*)

$BCl_4O_{16}^{\ominus}$ IC-000811

Tetraperchloratoborate(1 −), 8Cl
Tetrakis(perchlorato-O)borate(1 −), 10Cl, 9Cl
[62565-96-2]

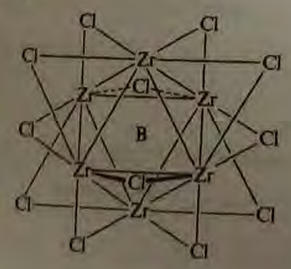
$[B(ClO_4)_4]^{\ominus}$

M 408.6 (ion)
NH_4 salt: [77951-42-9].
$BCl_4H_4NO_{16}$ M 426.6
Colourless solid.
▷ Stable at r.t. but stored cold in case of shock sensitive reaction.
Nitronium salt: [77951-43-0].
BCl_4NO_{18} M 454.6
Colourless solid.
▷ Stable at r.t. but stored cold in case of shock sensitive reaction.

Chausse, T. *et al, Nouv. J. Chim.*, 1981, **5**, 261 (*synth, ir, raman*)

$BCl_{13}Zr_6$ IC-000812

μ_6-Borylidynedodeca-μ-chlorochlorohexazirconium, 11Cl
Zirconium boride chloride (Zr_6BCl_{13})
[96929-13-4]



one Cl not shown

M 1019.0
One chlorine bridges to other $BCl_{12}Zr_6$ units. Synth. from Zr, $ZrCl_4$ and B in a sealed Ta tube at 700-860°. Black solid.

Ziebarth, R.P. *et al, J. Am. Chem. Soc.*, 1985, **107**, 4571 (*synth, cryst struct*)

$BCl_{12}Zr_6$ IC-000813

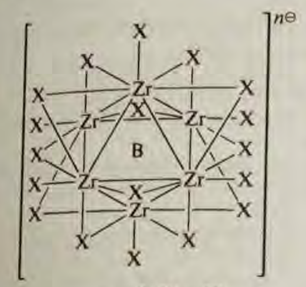
μ_6-Borylidynedodeca-μ-chlorodichlorohexazirconium, 11Cl
Zirconium boride chloride (Zr_6BCl_{14})
[96929-16-7]

M 1054.4
Two chlorines bridge to other $BCl_{12}Zr_6$ units; closely related to μ_6-Borylidynedodeca-μ-chlorochlorohexazirconium, IC-000812. Synth. from Zr, $ZrCl_4$ and B in a sealed Ta tube at 700-860°. Black solid.

Ziebarth, R.P. *et al, J. Am. Chem. Soc.*, 1985, **107**, 4571 (*synth, cryst struct*)

$BCl_{15}Zr_6^{1\ominus}$ IC-000814

μ_6-Borylidynedodeca-μ-chlorotrichlorohexazirconate(2 −), 11Cl



$n = 2, X = Cl$

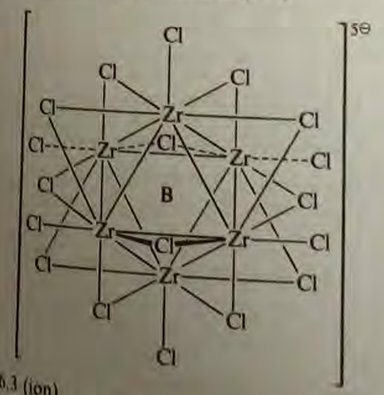
core cluster

M 1089.9 (ion)
Stoichiometry attained by extensive Cl-bridging between clusters.
Di-K salt: [96929-24-7].
Synth. by heating $ZrCl_4$, Zr, B and KCl in a sealed tube at 950°. Black cryst.

Ziebarth, R.P. *et al, J. Am. Chem. Soc.*, 1985, **107**, 4571; 1988, 110, 1132 (*synth, cryst struct*)

$BCl_{18}Zr_6^{5\ominus}$ IC-000815

μ_6-Borylidynedodeca-μ-chlorohexachlorohexazirconate(5 −), 12Cl
Hexazirconiumoctadecachloroboride(5 −)



M 1196.3 (ion)
Contains interstitial B atom in Zr_6 octahedron in isolated $[Zr_6BCl_{18}]^{5\ominus}$ anions.
Penta-Rb salt: [119878-69-2].
$BCl_{18}Rb_5Zr_6$ M 1623.6
Dark red cryst.

Ziebarth, R.P. *et al, J. Am. Chem. Soc.*, 1989, **111**, 3272 (*synth, cryst struct*)

[BCo]

Cobalt borides IC-000816

[12619-68-0]

A prep. of probably variable composition has been used in hydrogenations of olefins and acetylenes, as well as nitriles.

Cobalt boride* (Co_3B), *9Cl, 8Cl [12006-78-9]
Tricobalt monoboride
BCo_3 M 187.6
A metastable phase. Has Fe_3C (cementite) struct. Synth. from Co_2O_3 + B_4C + B. Mp 1280° (1125°) dec.

Cobalt boride* (Co_2B), *9Cl, 8Cl [12045-01-1]
Dicobalt monoboride
BCo_2 M 128.6
Synth. from Co_2O_3 + B_4C + B or CoS + BCl_3 under H_2 at <600°; Co_2O_3 + BN under NH_3 at 900°. Dec. at 845°.

Cobalt boride* (*CoB*), *9Cl, 8Cl [12006-77-8]
Cobalt monoboride
BCo M 69.7
FeB-type struct. Synth. from (i) Co_2O_3 + B_4C + C at 1000-1300°; (ii) B + C at 1100°; (iii) CoS + BCl_3 under H_2 at 600-800°; (iv) $NaBH_4$ + $CoCl_2$ at 350-400°. Mp 1460°. T_c 732K.

Cobalt boride* (CoB_2), *9Cl, 8Cl [11070-96-5]
Cobalt diboride
B_2Co M 80.5

Cueilleron, J. *et al, J. Less-Common Met.*, 1971, **24**, 317 (*synth, anal*)
Creel, R.B. *et al, J. Chem. Phys.*, 1972, **56**, 1549 (*nqr, cryst struct*)
Mavel, G. *et al, Surf. Sci.*, 1973, **35**, 109 (*pe*)
Sterlyadkina, Z.K. *et al, Zh. Neorg. Khim.*, 1973, **18**, 260; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 136 (*synth*)
Omari, S. *et al, Trans. Jpn. Inst. Metals*, 1976, **17**, 571; *CA*, **85**, 198935 (*phase diagram*)
Boron Refract. Borides, (Ed. Matkovich, V.I.,), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Aleshin, V.G. *et al, J. Less-Common Met.*, 1979, **67**, 173 (*pe*)
Bashev, V.F. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1981, **17**, 1206; *Inorg. Materials (Engl. Transl.)*, 1981, **17**, 892 (*synth*)
Ganem, B. *et al, Chem. Rev.*, 1986, **86**, 763 (*use, rev*)

[BCr] IC-000817

Chromium borides

In addition to phases described here, CrB_6 may exist.

Chromium boride* (Cr_4B), *9Cl, 8Cl [12006-81-4]
Tetrachromium boride
BCr_4 M 218.7
Mn_4B-type struct. Synth. from Cr_2S_3 + BCl_3 under H_2 at 800-1000°. Mp 1750° (1680°). Resistant to conc. HCl. Dissolved by H_2SO_4 + HNO_3.

Chromium boride* (Cr_2B), *9Cl, 8Cl [12006-80-3]
Dichromium monoboride
BCr_2 M 114.8
Mn_4B or $CuAl_2$-type structs. suggested. Existence in doubt. Mp 1875°.

Chromium boride* (Cr_3B_2), *9Cl, 8Cl [12007-38-4]
B_2Cr_3 M 292.4
Tetragonal lattice. Synth. from elements. Mp 2000°.

Chromium boride* (Cr_3B_2), *9Cl, 8Cl [12045-40-8]
Trichromium diboride
B_2Cr_3 M 177.6

Mp 2000° (1960°)

Chromium boride* (CrB), *9CI, 8CI [12006-79-0]

Chromium monoboride

BCr M 62.8

Orthorhombic with infinite zig-zag B atom chains which run through trigonal Cr atom lattice. Each B atom at centre of trigonal prism with Cr atom at each corner. Synth. from Cr_2O_3 + B at 1500° or from $CrCl_2$ + BCl_3 + H_2. Hard and metallic pillars. Mp ~2000°. Strongly paramagnetic. Stable at 1000-1300°.

Chromium boride* (Cr_3B_4), *9CI, 8CI [12045-71-5]

Trichromium tetraboride

B_4Cr_3 M 199.2

Ta_3B_4-type struct. Orthorhombic. Synth. from Cr_2O_3 + B at 1600° or from Cr + B. Thin plates or thick trapezoidal plates. Mp 1950°

Chromium boride* (Cr_2B_3), *9CI, 8CI [100629-17-2]

Dichromium triboride

B_3Cr_2 M 136.4

Orthorhombic lattice. Synth. from Cr + B in Al at > 1500°. Reacts with HF + HNO_3 + H_2SO_4 at 150°.

Chromium boride* (CrB_2), *9CI, 8CI [12007-16-8]

Chromium diboride

B_2Cr M 73.6

Hexagonal AlB_2-type struct. Also described as orthorhombic Mn_4B type. Synth. from Cr_2O_3 + B at 1600° or Cr_2O_3 + B_2O_3/Mg at 1200°, or BCl_3 + Cr_2S_3 under H_2 at 700-900°. Hard and metallic dendritic or hexagonal planar cryst. or hexagonal prisms. Mp 2130°. When finely divided, begins to oxidise in air at *ca.* 650°. Dissolves in H_2SO_4 aq. (1:2) and hot HNO_3. Stable to 5-20% NaOH aq., but added H_2O_2 accelerates dec. Attacked by fused NaOH.

[12653-35-3]

Gmelin Handbook Inorg. Chem., Syst. No. 52, 1962, **B**, 344 (*rev, bibl*)
Peshev, P. *et al, J. Less-Common Met.*, 1967, **13**, 241 (*synth, anal*)
Serebryakova, T.I. *et al, Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 3; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1 (*synth*)
Meerson, G.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 2075; *Inorg. Materials (Engl. Transl.)*, 1969, **5**, 1767 (*synth, purif*)
Markovskii, L.Ya. *et al, Poroshk. Metall. (Kiev)*, 1969, **9**, 13; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, **9**, 350 (*synth*)
Cueilleron, J. *et al, J. Less-Common Met.*, 1971, **24**, 317 (*synth*)
Marek, E.V. *et al, Poroshk. Metall. (Kiev)*, 1971, **11**, 70; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 138
Kugai, L.N., *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 769; *Inorg. Materials (Engl. Transl.)*, 1972, **8**, 669 (*props*)
Creel, R.B. *et al, J. Chem. Phys.*, 1972, **56**, 1549 (*nqr, cryst struct*)
Karasev, A.I. *et al, Poroshk. Metall. (Kiev)*, 1973, **12**, 1; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1973, **12**, 777 (*manuf*)
Mavel, G. *et al, Surf. Sci.*, 1973, **35**, 109 (*pe*)
Cruceanu, E. *et al, J. Less-Common Met.*, 1975, **41**, 339 (*synth, Cr_3B_4*)
Guy, C.N. *et al, J. Less-Common Met.*, 1976, **48**, 199 (*phase diagram, single cryst*)
Tanaka, T. *et al, J. Less-Common Met.*, 1976, **50**, 15 (*synth, single cryst, magnetic/electrical props*)
Boron Refract. Borides, (Ed. Matkovich, V.I.,), Springer-Verlag, Berlin, 1977, 361 (*rev, bibl*)
Kitaoka, Y. *et al, Solid State Commun.*, 1978, **26**, 87 (*B-11 nmr*)
Aleshin, V.G. *et al, J. Less-Common Met.*, 1979, **67**, 173 (*pe*)
Matojima, S. *et al, J. Crystal Growth*, 1981, **51**, 568 (*synth, single cryst, struct*)
Hamar, R. *et al, J. Crystal Growth*, 1983, **63**, 365 (*morphology*)
Okada, S. *et al, J. Solid State Chem.*, 1987, **68**, 61 (*cryst struct, CrB, Cr_3B_4, Cr_2B_3*)

$BCsH_8O_6$ IC-000818

Caesium metaborate tetrahydrate ($CsBO_2.4H_2O$)

Dicaesium diborate octahydrate

$Cs_2O.B_2O_3.8H_2O$ or $CsBO_2.4H_2O$

M 247.7

Colourless cryst. - known in α- and β-forms, latter previously thought to be a heptahydrate. Heating between 60-150° causes loss of six H_2O. Last two H_2O lost between 240-350°.

Lehmann, H.A. *et al, Z. Anorg. Allg. Chem.*, 1965, **335**, 50 (*synth, ir, thermal anal*)
Kocher, J., *Rev. Chim. Minér.*, 1966, **3**, 209 (*synth, thermal anal*)

[BDy] IC-000819

Dysprosium borides

DyB_2 has been reported in addition to the phases described here.

Dysprosium boride* (DyB_4), *9CI, 8CI [12310-43-9]

Dysprosium tetraboride

B_4Dy M 205.7

Tetragonal UB_4 struct.-type. Synth. from DyB_6 at high temp. Golden cryst. μ_{eff} = 10.4μ_B. Antiferromagnetic at low temp.

***Dysprosium boride* (DyB_6)** [12008-04-7]

Dysprosium hexaboride

B_6Dy M 227.3

Has the cubic CaB_6-type struct. Synth. from Dy_2O_3 + B at 1500-1600° or Dy_2O_3 + B_2O_3 + Mg at 1200°. Light blue solid becoming darker in colour when heated in air. Mp 1220°. Sol. HNO_3 at r.t., but stable to hot HCl (1:2). Reacts with H_2O at 300° under pressure. Reactive to H_2O_2.

▷ Thermally stable to 650-700° but pyrophoric as fine powder, and ignites at 730°.

Dysprosium boride* (DyB_{12}), *9CI, 8CI [12589-34-3]

Dysprosium dodecaboride

$B_{12}Dy$ M 292.2

Cubic UB_{12}-type struct. Synth. from Dy_2O_3 + B at 1450-1600°. Less reactive than lower borides. Resists HCl, H_2SO_4 and dec. only by oxidising acids (H_2SO_4 + HNO_3, cold HNO_3, aqua regia). At high temp. dissociates to DyB_6.

Dysprosium boride* (DyB_{66}), *9CI [11141-33-6]

$B_{66}Dy$ M 876.0

Struct. has B_{12} icosahedron surrounded by 12 B_{12} linked icosahedra. Unit cell has 1584 B atoms and 24 Dy atoms. Synth. from elements. Mp *ca.* 2150°. Refractory. V. hard.

Timofeeva, N.I. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1789; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1559 (*synth*)
Timofeeva, N.I. *et al, Zh. Prikl. Khim. (Leningrad)*, 1969, **42**, 2339; *J. Appl. Chem. USSR (Engl. Transl.)*, 1969, **42**, 2194 (*synth, props*)
Yukhimenko, E.V. *et al, Poroshk. Metall. (Kiev)*, 1971, **11**, 52; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 895 (*anal, props*)
Timofeeva, E.N. *et al, Zh. Prikl. Khim. (Leningrad)*, 1971, **44**, 1400; *J. Appl. Chem. USSR (Engl. Transl.)*, 1971, **44**, 1414 (*props*)
Buschow, K.H.J. *et al, J. Chem. Phys.*, 1972, **57**, 3910 (*magnetism*)
Schwetz, K. *et al, J. Less-Common Met.*, 1972, **26**, 99 (*synth, cryst struct*)
Fisk, Z. *et al, Mater. Res. Bull.*, 1972, **7**, 285 (*cryst struct*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.,), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Schäfer, W *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1977, **144**, 217 (*nd, struct*)

Dudnik, E.M. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1979, **15**, 627; *Inorg. Materials (Engl. Transl.)*, 1979, **15**, 490 (*synth*)
Will, G. *et al, J. Less-Common Met.*, 1979, **67**, 31 (*nd, struct*)
Fisk, Z. *et al, Solid State Commun.*, 1981, **39**, 1189 (*magnetism*)
Golikova, O.A. *et al, J. Non-Cryst. Solids*, 1986, **87**, 64 (*electrical, opt props*)

BDy_2Fe_{14} IC-000820

Dysprosium iron boride ($Dy_2Fe_{14}B$)

[94186-33-1]

$Dy_2Fe_{14}B$

M 1117.6

Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. Magnetic recording material. T_c 590K. Absorbs hydrogen.

Andreev, A.V. *et al, Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)
Herbst, J.F. *et al, J. Appl. Phys.*, 1985, **57**, 2343 (*nd, cryst struct, magnetism*)
Pinkerton, F.E. *et al, J. Appl. Phys.*, 1985, **57**, 4121 (*mössbauer*)
Dub, O.M. *et al, CA*, 1986, **105**, 201912 (*synth, cryst struct*)

[BEr] IC-000821

Erbium borides

In addition to phases described here, the diboride has also been reported.

Erbium boride* (ErB_4), *9CI, 8CI [12310-44-0]

Erbium tetraboride

B_4Er M 210.5

Tetragonal UB_4-type struct. becoming orthorhombic at 15K. Golden cryst. μ_{eff} = 8.98 (9.52)μ_B. Antiferromagnetic in weak field becoming ferromagnetic at higher fields.

Erbium boride* (ErB_6), *9CI, 8CI [12046-33-2]

B_6Er M 232.1

Cubic CaB_6-type struct. Blue solid.

Erbium boride* (ErB_{12}), *9CI, 8CI [12589-35-4]

Erbium dodecaboride

$B_{12}Er$ M 296.9

Cubic UB_{12}-type struct. Synth. from Er_2O_3 + B when heated at 1500-1700°. Mp 2082°. More resistant to oxidation than Er metal. Resistant to HCl, H_2SO_4, and dec. only by oxidising acids (aq. regia, HNO_3).

Erbium boride* (ErB_{66}), *9CI [37322-39-7]

$B_{66}Er$ M 880.7

Struct. has B_{12} icosahedron surrounded by 12 B_{12} linked icosahedra. Unit cell contains 1584 B atoms and 24 Er atoms. Synth. from elements. Mp *ca.* 2150°. V. hard and refractory.

Yukhimenko, E.V. *et al, Poroshk. Metall. (Kiev)*, 1971, **11**, 52; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 895.
Buschow, K.H.J. *et al, J. Chem. Phys.*, 1972, **57**, 3910 (*magnetism*)
Schwetz, K. *et al, J. Less-Common Met.*, 1972, **26**, 99 (*synth*)
Fisk, Z. *et al, Mater. Res. Bull.*, 1972, **7**, 285 (*cryst struct*)
Paderno, Yu.B. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, **10**, 1900; *Inorg. Materials (Engl. Transl.)*, 1974, **10**, 1633 (*magnetism*)
Ames, L.L. *et al, High Temp. Sci.*, 1975, **7**, 44 (*ms*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.,), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Schäffer, W. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1977, **144**, 217 (*cryst struct*)
Bressel, B. *et al, J. Crystal Growth*, 1979, **47**, 429 (*cryst struct*)
Will, G. *et al, J. Less-Common Met.*, 1979, **67**, 31; 1981, **82**, 349 (*nd, cryst struct, magnetism*)
Etourneau, J. *et al, J. Less-Common Met.*, 1979, **67**, 531 (*magnetic, electrical props*)
Will, G. *et al, Rev. Chim. Minér.*, 1980, **17**, 533 (*nd, struct*)
Odintsov, V.V. *et al, Poroshk. Metall. (Kiev)*, 1984, **23**, 71; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1984, **23**, 68 (*props*)
Hieba, Z. *et al, J. Phys. Chem. Solids*, 1986, **47**, 651 (*struct, magnetic props*)

[BEu] IC-000822

Europium borides

[103370-73-6]

Borides < EuB_6 not observed.

Europium boride* (EuB_6), *9CI, 8CI [12008-05-8]

Europium hexaboride

B_6Eu M 216.8

Possesses the cubic CaB_6-type struct. with Eu(*II*) oxidation state. Synth. from Eu_2O_3 + H_3BO_3 + Mg at 1100°. Neutron absorber for fast reactors. Bluish solid. Mp 2660° (2580°). Semiconductor. Becomes ferromagnetic at <15K. Vaporises to elements. μ_{eff} = 8.1μ_B.

▷ Pyrophoric in dry or moist air (700-750°).

Markovskii, L.Ya. *et al, Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1824; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1752 (*synth*)
Timofeeva, N.I. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1789; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1559 (*synth, props*)
Ryabchikov, D.I. *et al, Zh. Neorg. Khim.*, 1968, **13**, 588; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 304 (*props*)
Mordovin, O.A. *et al, Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Savitskii, E.M. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 617; *Inorg. Materials (Engl. Transl.)*, 1971, **7**, 539 (*synth, phase diagram*)
Schwetz, K. *et al, J. Less-Common Met.*, 1973, **33**, 295 (*synth, cryst struct*)
Ames, L.L. *et al, High Temp. Sci.*, 1975, **7**, 44 (*ms*)
Mercurio, J.P. *et al, J. Less-Common Met.*, 1976, **47**, 175 (*electrical props, magnetism*)
Ishii, M. *et al, Solid State Commun.*, 1976, **20**, 437 (*synth, raman*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.,), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Tanaka, T. *et al, J. Crystal Growth*, 1977, **40**, 125 (*synth, single cryst*)
Volkonskaya, T.I. *et al, Fiz. Tverd. Tela (Leningrad)*, 1979, **21**, 631; *Soviet Physics: Solid State*, 1979, **21**, 375 (*magnetism*)
Reinmuth, K. *et al, J. Nucl. Mater.*, 1984, **124**, 175 (*use*)

BFH_2 IC-000823

Fluoroborane

Fluoroborine. Fluorodihydroboron

[27944-03-2]

H_2BF

M 31.8

Not prepd. in pure form, but known in a variety of complexes.

$MeNH_2$ complex: [67194-41-6]. *Fluorodihydro(methylamine) boron*

CH_7BFN M 62.8

Substantially more stable than Me_3N complex.

Me_2NH complex: [67194-40-5].

Fluorodihydro(dimethylamine)boron

C_2H_9BFN M 76.9

More stable than Me_3N complex.

Me_3N complex: [35449-24-2]. *Fluorodihydro(trimethylamine) boron*

$C_3H_{11}BFN$ M 90.9

Mp 117-118°.

Me_3P complex: [67226-44-2]. *Fluorodihydro(trimethylphosphine)boron, (9CI*

$C_3H_{11}BFP$ M 107.9
Less stable than Me_3N complex.
Ph_2P complex: (67194-38-1].
Fluorodihydro(triphenylphosphine)boron, 10Cl
$C_{18}H_{17}BFP$ M 294.1
Much less stable than the Me_3N complex.

Walsh, A.D., *J. Chem. Soc.*, 1953, 2260 (*struct*)
Van Paasschen, J.M. *et al, Inorg. Nucl. Chem. Lett.*, 1972, **8**, 879.
Dill, J.D. *et al, J. Am. Chem. Soc.*, 1975, **97**, 3402.
Van Paasschen, J.M. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 2321.
Van Paasschen, J.M. *et al, Inorg. Chem.*, 1978, **17**, 3302.
Bernardi, F. *et al, J. Am. Chem. Soc.*, 1978, **100**, 7205.
Cassioux, P. *et al, J. Mol. Struct.*, 1978, **48**, 25 (*microwave*)
Hinde, A.L. *et al, J. Comput. Chem.*, 1980, **1**, 118.

IC-000824

BF_2H

Difluoroborane, 10Cl, 9Cl
Difluoroborine
[13709-83-6]

F_2BH

M 49.8
Prototype of the alkyldifluoroborane series of compds. Prepd. from solid boroxine and BF_3 (gas). Air- and moisture-sensitive gas. ΔH_f° – 736 kJ mol^{-1}

Mikhailov, B.M. *et al, Zh. Obshch. Khim.*, 1959, **29**, 3443 (*use*)
Coyle, T.D. *et al, Proc. Chem. Soc., London*, 1964, 25 (*synth*)
Porter, R.F. *et al, J. Phys. Chem.*, 1965, **69**, 2208 (*synth*)
Tuzhagues, J.P. *et al, J. Organomet. Chem.*, 1973, **54**, 69 (*ir, nmr*)
Dimofano, A.J. *et al, Thermochim. Acta*, 1976, **16**, 236 (*use*)
Fussstetter, H. *et al, Chem. Ber.*, 1977, **110**, 3172 (*nmr*)

IC-000825

BF_3

Boron trifluoride
Trifluoroborane, 11Cl, 10Cl, 9Cl, Boron fluoride (BF_3), 8Cl
[7637-07-2]

BF_3 (D_{3h})

M 67.8
B—F 131.3 pm (gas phase by ed and ir). Lewis acid; forms many adducts with O,S,N,P-donors. Synth. by heating CaF_2, B_2O_3 + conc. H_2SO_4; or by dehydration of $B(OH)_3$ in presence of PhCOF. Commercially available. Catalyst for many org. reactions eg. Friedel-Crafts reactions, polymerisations, carbonylations. Colourless, non-flammable gas. Sol. H_2O, org. solvs. eg. alcohols, ethers (forming adducts). Mp – 128.4°. Bp – 100.0°. ΔH_f° – 1135.9 kJ mol^{-1}.

▷ Toxic, irritant gas, slowly hydrol. to give HF. ED2275000.

Et_2O complex: [109-63-7]. *(Diethyl ether)trifluoroboron. Trifluoro[1,1'-oxybis[ethane]]boran, 10Cl. 1,1'-Oxybis[ethane] compd. with trifluoroborane (1:1), 9Cl. Ethyl ether compd. with boron fluoride (BF_3) (1:1), 8Cl. Trifluoroborane etherate. Boron trifluoride etherate*
$C_4H_{10}BF_3O$ M 141.9
V. important catalyst for many types of reactions. Lewis acid. Commercially available. Moisture-sensitive liq.
Misc. ethers, CH_2Cl_2. d^{25} 1.125. Mp – 58°. Bp 126°. n_D^{25} 1.348.

▷ Corrosive. KX7375000.

Monohydrate: see *Aquatrifluoroboron, IC-000827*
NH_3 complex: [13709-86-9]
BF_3H_4N M 84.8

CO complex: see *Carbonyltrifluoroboron, IC-002276*
Me_2O complex: see *(Dimethyl ether)trifluoroboron, IC-003165*
Py complex: see *Trifluoro(pyridine)boron, IC-004680*

Steinhardt, R.G. *et al, J. Chem. Phys.*, 1965, **43**, 4528 (*ir, raman*)
Kuchitsu, K. *et al, J. Chem. Phys.*, 1966, **45**, 4342 (*ed, gas phase struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 70; 1969, **2**, 35; 1972, **3**, 33; 1974, **4**, 44; 1975, **5**, 54; 1977, **6**, 65; 1979, **7**, 31; 1980, **8**, 51; 1981, **9**, 64; 1982, **10**, 52; 1984, **11**, 72 (*uses*)
Gillespie, R.J. *et al, Can. J. Chem.*, 1968, **46**, 2147 (*F-19 nmr*)
Fratiello, A. *et al, J. Am. Chem. Soc.*, 1968, **90**, 1194 (*nmr, pmr*)
Fratiello, A. *et al, Inorg. Chem.*, 1969, **8**, 480 (*nmr*)
Topchii, V.A. *et al, Zh. Obshch. Khim.*, 1969, **39**, 2689 (*deriv*)
Bassett, P.J. *et al, J. Chem. Soc., Chem. Commun.*, 1970, 36 (*pe*)
Lappert, M.F. *et al, J. Chem. Soc. A*, 1971, 2426 (*B-11 nmr*)
Murphy, C.B. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 1622 (*ms*)
Fratiello, A. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 93 (*pmr, cmr*)
Voloshchuk, A.M. *et al, Kernenergie*, 1974, **17**, 121 (*ir, deriv*)
Beattie, W.H., *Appl. Spectrosc.*, 1975, **29**, 334 (*ms*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, 1978, **19**, 35 (*rev, manuf, props*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 685 (*rev, props, uses*)
Sugawara, T. *et al, Bull. Chem. Soc. Jpn.*, 1979, **52**, 3391 (*deriv, nmr*)
Hunt, R.L. *et al, Spectrosc. Int. J.*, 1982, **1**, 31 (*matrix, ir, NH_3 complex*)
Binbrek, O.S. *et al, Can. J. Spectrosc.*, 1983, **28**, 173 (*raman, solid*)
Colquhoun, H.M. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 63 (*cryst struct, NH_3 complex*)

IC-000826

$BF_3H^\ominus$

Trifluorohydroborate(1 –), 9Cl
Trifluoroborohydride
[57384-26-6]

$[BF_3H]^\ominus$

M 68.8 (ion)
Li salt: [52082-04-9]. *Lithium trifluorohydroborate. Lithium trifluoroborohydride*
BF_3HLi M 75.7
Colourless solid. Sol. MeCN, Me_2CO, DMSO. Reacts with H_2O, alcohols.

Goubeau, J. *et al, Z. Anorg. Allg. Chem.*, 1950, **263**, 69 (*synth, powder struct*)
Buslaev, Yu.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1973, **213**, 1349 (*synth, F-19 nmr*)
Mazitov, R.K. *et al, Theor. Exp. Chem. (Engl. Transl.)*, 1975, **11**, 336; *CA*, **83**, 123709 (*Li-7, B-11, F-19 nmr*)

IC-000827

BF_3H_2O

Aquatrifluoroboron
Trifluoroborane monohydrate, 11Cl, 10Cl, 9Cl. Boron fluoride monohydrate, 8Cl. Boron trifluoride hydrate. Hydrogen trifluorohydroxyborate. Boron trifluoride-water complex (1:1)
[15799-89-0]

$F_3B{-}OH_2$ or $H[F_3B(OH)]$

M 85.8
Has a molecular form in slowly crystallised solid state but an ionic form if cooled quickly, or in liq. state. Used as catalyst in carbonylation of olefins. Colourless liq.; dec. >15°. Sol. H_2O (slow hydrol.). Mp 5.9-6°. d^{20} 1.786.

Monohydrate: [13319-75-0].
$BF_3H_4O_2$ M 103.8
▷ ED2285000.

Greenwood, N.N. *et al, J. Chem. Soc.*, 1951, 1915 (*synth, props*)
Ford, P.T. *et al, J. Chem. Soc.*, 1956, 3870 (*pmr, F-19 nmr*)
Bates, J.B. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 2721 (*ir*)

Mootz, D. *et al, Acta Crystallogr., Sect. B*, 1981, **37**, 1110 (*cryst struct, deriv*)
Mootz, D. *et al, Z. Anorg. Allg. Chem.*, 1981, **483**, 171 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *Suppl.*, 1987, **3** (*uses*)

IC-000828

BF_3H_3P

Trihydro(trifluorophosphine)boron
Trifluorophosphine borane (1:1), 9Cl. Borane trifluorophosphine. Borane compd. with phosphorus trifluoride
[14931-39-6]

$H_3B{-}PF_3$

M 101.8
Interatomic distances: B—H 120.7, P—F 153.8, P—B 183.6 pm; angles: HBH 115°, FPF 100°. Synth. from PF_3 + BH_3 in sealed tube at r.t. Colourless gas. Mp –116°. Bp –61.6° (extrap.). Suffers 14% dec. in 1 hr. at r.t.

▷ Spont. flammable.

Parry, R.W. *et al, J. Am. Chem. Soc.*, 1956, **78**, 1524 (*synth, props*)
Deever, W.R. *et al, J. Am. Chem. Soc.*, 1967, **89**, 5073 (*synth, ir, props*)
Kuczkowski, R.L. *et al, J. Chem. Phys.*, 1967, **46**, 357 (*microwave*)
Cowley, A.H. *et al, J. Am. Chem. Soc.*, 1971, **93**, 6815 (*pmr, B-11 nmr*)
Labarre, J.F. *et al, Int. J. Quantum Chem.*, 1972, **6**, 625 (*conform*)
Jouany, C. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1974, **71**, 395 (*B-11 nmr, P-31 nmr*)
Odom, J.D. *et al, J. Mol. Struct.*, 1974, **20**, 471 (*ir, raman*)

IC-000829

$BF_4^\ominus$

Tetrafluoroborate(1 –), 11Cl, 10Cl, 9Cl, 8Cl
[14874-70-5]

$[BF_4]^\ominus$

M 86.8 (ion)
Na salt: see *Sodium tetrafluoroborate ($NaBF_4$), IC-000833*
K salt: see *Potassium tetrafluoroborate (KBF_4), IC-000831*
H compd.: see *Tetrafluoroboric acid, IC-000830*
NH_4 salt: [13826-83-0]. *Ammonium tetrafluoroborate*
BF_4H_4N M 104.8
Colourless cryst.
▷ BQ6100000.

Nitrosyl salt: [14635-75-7]. *Nitrosyl tetrafluoroborate*
BF_4NO M 116.8
Commercially available – used in org. and organomet. chem. as source of NO groups. Colourless cryst., easily hydrol. Sol. MeCN. Subl. without dec.

Nitronium salt: [13826-86-3]. *Nitryl salt*
BF_4NO_2 M 132.8
Used in nitration of org. compds. Colourless cryst.; easily hydrol. Spar. sol. MeCN, $MeNO_2$. Strong oxidising agent.
▷ QX8620000.

Triethyloxonium salt: see *Triethyloxonium tetrafluoroborate, IC-005215*
[34216-27-8]

Cook, D. *et al, J. Chem. Phys.*, 1960, **33**, 1669 (*synth, ir*)
Evans, J.C. *et al, Inorg. Chem.*, 1964, **3**, 857 (*ir*)
Nöth, H. *et al, Chem. Ber.*, 1966, **99**, 1049 (*B-11 nmr*)
Org. Synth., Coll. Vol., 5, 1973, 480, 1080 (*rev, bibl, synth*)
Akitt, J.W., *J. Chem. Soc., Faraday Trans. 1*, 1975, **71**, 1557 (*F-19 nmr*)
Sergienko, V.I. *et al, Koord. Khim.*, 1977, **3**, 480; *CA*, **87**, 13696 (*ir*)
Jones, F.R. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 927 (*synth, pmr, thermal anal*)

BF_4H

IC-000830

Tetrafluoroboric acid
Fluoroboric acid. Hydrofluoroboric acid. Hydrogen tetrafluoroborate, 11Cl, 10Cl, 9Cl, 8Cl
[16872-11-0]

$H[BF_4]$

M 87.8
Usually refers to acidified solns. of $[BF_4]^\ominus$ ions. Commercially available as 48% aq. HBF_4 soln. Reagent for fluoroborate salt prep. Used in metal finishing and electrochemistry. Sol. H_2O. pK_a –4.9. Aq. solns. hydrol. to B—OH containing species.

▷ Reacts with glass. ED2685000.

Bonadeo, H. *et al, J. Mol. Spectrosc.*, 1969, **32**, 214 (*ir*)
Mesmer, R.E. *et al, Inorg. Chem.*, 1973, **12**, 699 (*F-19 nmr*)
Akitt, J.W., *J. Chem. Soc., Faraday Trans. 1*, 1975, **71**, 1557 (*F-19 nmr, B-11 nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 693 (*manuf, uses*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *Suppl. Vol.*, 1982, **2**: 1988, **3** (*rev, bibl*)

BF_4K

IC-000831

Potassium tetrafluoroborate (KBF_4)
Potassium fluoborate. Potassium borofluoride. Tetrafluoroborate, potassium salt
[14075-53-7]

KBF_4

M 125.9
Synth. by reaction of excess B_2O_3 with KCl and BrF_3. Commercially available. Used to harden steel (boronisation) and as a component of brazing fluxes. Colourless orthorhombic cryst. Undergoes orthorhombic to cubic transition at 283°. Sl. sol. H_2O (0.4 g per 100 cm^3 at 20°; 6.3 g per 100 cm^3 at 100°); spar. sol. Et_2O, EtOH. Mp 570°. ΔH_f° –1887 kJ mol^{-1}; ΔG_f° –1785 kJ mol^{-1}; S° 134 J K^{-1} mol^{-1}.

▷ Corrosive. ED2800000.

Mineral-form [1303-68-0]
Avogadrite
Contains Cs: $(K,Cs)BF_4$. Sublimation product at Mt. Vesuvius. Minute cryst.

[12197-25-0]

Finbak, C. *et al, Z. Phys. Chem. (Leipzig), Abt. B*, 1936, **32**, 433 (*polymorphs*)
Woolf, A.A. *et al, J. Chem. Soc.*, 1950, 1050 (*synth*)
Clark, M.J.R. *et al, Can. J. Chem.*, 1969, **47**, 2579 (*struct*)
Bates, J.B. *et al, Spectrochim. Acta, Part A*, 1975, **31**, 1317 (*ir, raman*)
Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 215 (*thermochem data, polymorphs*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2911A (*haz*)

IC-000832

BF_4Li

Lithium tetrafluoroborate(LiBF$_4$)
Tetrafluoroborate(1 –), lithium salt, 8Cl
[14283-07-9]

$LiBF_4$

M 93.7
Synth from LiF + BF_3 in THF or 1,2-dimethoxyethane. Commercially available as solid or in soln. (1.0 *M*) in MeCN. Electrolyte for use in non-aq. lithium batteries. Reagent for the cleavage of silyl ethers, the mild high yield hydrolysis of acetals and ketals, the addition of arenesulfonyl chlorides to olefins and the electrooxidative C—C cleavage of cyclohexanones. Hygroscopic. Dec. on heating into constituent fluorides (dissociation pressure ~ 675 mm Hg at 300°). ΔH_f° −1876 kJ mol^{-1}; ΔG_f° −1777 kJ mol^{-1}.

▷ Irritant.

Monohydrate: [39863-03-6].
BF_4H_2LiO M 111.7
Colourless orthorhombic cryst.

Trihydrate: [39863-05-8].
Colourless hexagonal cryst. Dec. at 23° with H_2O loss to give monohydrate.

Gmelin Handbook Inorg. Chem., Syst. No. 20, 1980, 493 (rev, bibl)
Murawec, M. *et al, Z. Naturforsch., B*, 1932, **27**, 1127 (*ir, raman, bibl*)
Sergienko, V.I. *et al, Koord. Khim.*, 1977, **3**, 480 (*ir*)
Kanai'an, A.S. *et al, High Temp. Sci.*, 1979, **11**, 23 (*thermal dec*)
Mirzoff, R.W. *et al, Tetrahedron Lett.*, 1980, **21**, 35 (*uses*)
Zubrov, N.S. *et al, J. Org. Chem.*, 1981, **46**, 5264 (*uses*)
Japan. Pat., 81 145 113, (1981); *CA*, 1982, **96**, 126323 (*synth*)
Tori, S. *et al, J. Org. Chem.*, 1982, **47**, 47 (*uses*)
Lipshutz, B.H. *et al, Synth. Commun.*, 1982, **12**, 267 (*uses*)
Vasilcina, T.F. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1986, **31**, 1313 (*cryst struct, biblio*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2158A

BF_4Na IC-000833
Sodium tetrafluoroborate ($NaBF_4$)
Sodium fluoborate, 8CI. Sodium borofluoride
Tetrafluoroborate, sodium salt
[13755-29-8]

$NaBF_4$

M 109.7
Synth. either by neutralisation of NaOH or Na_2CO_3 with aq. HBF_4 (excess HF) or by reaction of BF_3 with NaF. Alternatively HF can be absorbed in aq. borax to produce $NaBF_4$ directly. Commercially available. Used in the electroplating industry. Grain refining agent for aluminium. White orthorhombic cryst. Dec. on heating >200° to form NaF and BF_3. V. sol. H_2O (108 g per 100 cm^3 at 26°; 210 g per 100 cm^3 at 100°); spar. sol. EtOH. Mp 322°

▷ Corrosive. ED2975000.

Mineral-form [24203-02-9]
Fersuvite
Occurs as a sublimation product around fumaroles on Mt. Vesuvius. Minute tabular cryst.

Cont. G.L. et al, Proc. R. Soc. London, A, 1951, **210**, 217 (*ir*)
Edwards, J.O. *et al, J. Am. Chem. Soc.*, 1955, **77**, 266 (*raman*)
Otuk, T.P. *et al, J. Phys. Chem.*, 1959, **63**, 1533 (*B-11 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1966, **3**, 1305 (*rev, bibl*)
Hohne, E. *et al, Z. Anorg. Allg. Chem.*, 1966, **344**, 179 (*cryst struct*)
Epperlein, B.W. *et al, Z. Naturforsch., A*, 1975, **30**, 955 (*B-10, B-11 nmr*)
Stepenko, V.I. *et al, Zh. Struk. Khim.*, 1979, **20**, 957 (*F-19 nmr*)
Tabeta, R. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3158A (*bibl*)

BF_4Tl IC-000834
Thallium(*I*) tetrafluoroborate
[28625-02-7]

$Tl[BF_4]$

M 291.1
Isostructural with barite structure - orthorhombic; transforms to cubic at 201.7°. Synth. from 40% fluoroboric acid + Tl_2CO_3. Colourless, moisture-sensitive solid. Spar. sol. H_2O.

▷ Highly toxic. ED3150000.

Yeager, H.L. *et al, J. Phys. Chem.*, 1970, **74**, 963 (*synth*)
Pistorius, C.W.F.T., *Z. Anorg. Allg. Chem.*, 1970, **376**, 308 (*struct*)
Clark, J.B. *et al, J. Solid State Chem.*, 1973, **7**, 353 (*struct*)

BF_3OSi IC-000835
Difluoro[(trifluorosilyl)oxy]borane, 11CI
[80274-63-1]

$F_3Si—O—BF_2$

M 149.8

Glidewell, C., *J. Mol. Struct.*, 1981, **85**, 373 (*theory*)

BF_5Si IC-000836
Difluoro(trifluorosilyl)borane, 11CI, 9CI, 8CI
[19091-19-1]

F_3SiBF_2

M 133.8
Air sensitive, stable at r.t.

Smith, D.L. *et al, J. Chem. Soc., Chem. Commun.*, 1972, 295 (*synth, ir, B-11 nmr, F-19 nmr, ms*)
Langridge-Smith, P.R.R. *et al, J. Chem. Soc., Faraday Trans. 2*, 1983, **79**, 1089 (*microwave, struct*)

$BF_6H_2Si_2^{\ominus}$ IC-000837
Dihydrobis(trifluorosilyl)borate(1−), 10CI

$[(F_3Si)_2BH_2]^{\ominus}$

M 182.9 (ion)

Tetrabutylammonium salt: [74354-31-7].
Not isol. Sol. CH_2Cl_2.

Brownstein, S., *J. Chem. Soc., Chem. Commun.*, 1980, 149 (*synth, pmr, B-11 nmr, F-19 nmr*)

$BF_{10}O_3Te_3$ IC-000838
Tris[pentafluorotellurato(*VI*)]boron
Tris[pentafluorotellurato(VI)]borane. Boron tris[pentafluorotellurate(VI)]. Tellurium borate fluoride ($Te_3(BO_3)F_{15}$)
[40934-88-1]

$B(OTeF_5)_3$ (D_{3h})

M 726.5
B in planar environment. Synthesis: BCl_3 + $3TeF_5OH$ at −80°. Lewis acid comparable to BCl_3. Reagent for introduction of -$OTeF_5$ group. Colourless cryst., readily hydrol., subl. at r.t. *in vacuo*. Sol. CCl_3F, $PhNO_2$, relat. solvs. Mp 37°. Dec. >140°.

Sladky, F. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 134 (*synth, ms, ir, F-19 nmr, thermochem, deriv*)
Sawyer, J.F. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 1561 (*cryst struct*)

$BFe_{0.8}Ni_{0.2}$ IC-000839
Iron-nickel-boron alloys

(Fe,Ni)B

M 68.0
Listed here under sample formula. Prepd. from constituent elements of high purity with rapid quenching from the melt. Used in transformer cores. An amorphous ferromagnet. There is only a small difference in moment (<5%) between the cryst. and amorphous forms.

O'Handley, R.C. *et al, Appl. Phys. Lett.*, 1976, **29**, 330 (*synth, ferromagnetism*)
Luborsky, F.E., *Ferromagnetic Materials*, North-Holland, Amsterdam, 1980, **1**, 451.
Balogh, J. *et al, J. Phys. Colloq.*, 1980, 255 (*struct*)

[BFe] IC-000840
Iron borides
[39383-96-5]

Iron boride (Fe_3B), 9CI, 8CI [12006-86-9]
Trilron monoboride
BFe_3 M 178.3
Metastable orthorhombic and tetragonal phases of sl. different stoichiometries; orthorhombic form is essentially isostruct. with Fe_3C (cementite). T_c 800K. Highly unstable.

Iron boride (Fe_2B), 9CI, 8CI [12006-85-8]
Dilron monoboride
BFe_2 M 122.5
Tetragonal lattice of the $CuAl_2$-type. Sol. HNO_3, HCl aq. (1:1), H_2SO_4 (1:1) and $HClO_4$. Reacts with boiling H_2O. Mp 1390°. Ferromagnetic. μ_{eff} = 1.91μ_B; T_c 1013K.

Iron boride (FeB), 9CI, 8CI [12006-84-7]
Iron monoboride. Iron(III) boride
BFe M 66.6
Orthorhombic cell with each B atom surrounded by 6 Fe atoms at vertices of a trigonal prism; B atoms form infinite chains. Basic struct. is hcp. Synth. from FeS + BCl_3 under H_2 at >500°; or from $FeCl_2$ aq. + $NaBH_4$. Hydrogenation catalyst. Sol. dil. and conc. HNO_3, conc. and 1:1 HCl aq., H_2SO_4 (1:1) and $HClO_4$. Mp 1540°. μ_{eff} = 1.11μ_B. Exists in low temp. α-form and higher temp. β-form with identical T_c (602K) α→β with change in magnetic moment. Both forms ferromagnetic. Reacts with boiling H_2O.

Iron boride (FeB_2), 9CI, 8CI [12007-18-0]
B_2Fe M 77.4
Reported to exist in Fe-B alloys. Mp 1410°.

[60581-41-1]

Wessman, I.D. *et al, Phys. Rev.*, 1969, **177**, 465 (*cryst struct, B-11 nmr, mössbauer*)
Timofeeva, N.I. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 1619; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 1423 (*props*)
Cuilleron, J. *et al, J. Less-Common Met.*, 1971, **24**, 317 (*synth*)
Kunitskii, Yu.A. *et al, Poroshk. Metall. (Kiev)*, 1971, **11**, 56; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 216 (*rev, phys props*)
Mavel, G. *et al, Surf. Sci.*, 1973, **35**, 109 (*pe*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Choo, W.K. *et al, Metall. Trans. A*, 1977, **8**, 417 (*mössbauer, struct*)
Alechin, V.G. *et al, J. Less-Common Met.*, 1979, **67**, 173 (*pe*)
Chien, C.L. *et al, Phys. Rev. B*, 1979, **20**, 283; 1984, **29**, 207 (*magnetism, synth, struct, mössbauer*)
Joyner, D.J. *et al, J. Am. Chem. Soc.*, 1980, **102**, 1910 (*pe, struct*)
Pokatilov, V.S., *Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1981, **257**, 95; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1981, **26**, 327 (*B-11 nmr*)
Bashev, V.F. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1981, **17**, 1206; *Inorg. Materials (Engl. Transl.)*, 1981, **17**, 892.
Le Caer, G. *et al, Phys. Status Solidi A*, 1981, **64**, 275 (*mössbauer, struct*)
Kanaizuka, T., *Phys. Status Solidi A*, 1982, **69**, 739 (*synth, mössbauer, magnetism*)
Matz, W. *et al, Phys. Status Solidi A*, 1983, **76**, K17 (*nd, struct*)

$BFeO_3$ IC-000841
Iron(*III*) borate ($FeBO_3$)
Iron(III) trioxoborate(III)

$FeBO_3$

M 114.6
Isostructural with calcite.

Oxide: [12228-26-1]. *Iron borate oxide ($Fe_3(BO_3)O_2$)*
BFe_3O_5 M 258.3
Used in boronised high-speed cutting tools.
Oxide: see *Iron(III) borate oxide ($Fe_3(BO_3)O_3$), IC-000842*
Diehl, R., *Solid State Commun.*, 1975, **17**, 743 (*struct*)
Muellerwiebus, E.U. *et al, Physica B+C (Amsterdam)*, 1977, **86-88**, 1261 (*magnetism*)
Farmer, J.B., *Adv. Inorg. Chem. Radiochem.*, 1982, **25**, 187 (*rev, bibl*)

BFe_3O_6 IC-000842
Iron(*III*) borate oxide ($Fe_3(BO_3)O_3$)
[12446-83-2]

$Fe_3(BO_3)O_3$

M 274.3
Struct. based on sl. distorted hcp O atoms; B is tetrahedrally coord. to 4 O atoms. Synth. from B_2O_3 + Fe_2O_3 at 850°. Used in ceramic coatings. Black prismatic cryst.; ferrimagnetic. T_N 235°.

Diehl, R. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 1662 (*struct*)
Muellerwiebus, E.U. *et al, Physica B+C (Amsterdam)*, 1977, **86-88**, 1261 (*magnetism*)
Farmer, J.B., *Adv. Inorg. Chem. Radiochem.*, 1982, **25**, 187 (*rev, bibl*)

$BFe_{14}Gd_2$ IC-000843
Gadolinium iron boride ($Gd_2Fe_{14}B$)
[93388-50-2]

$Gd_2Fe_{14}B$

M 1107.1
Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. Important in magnet technology. T_c 662K. Absorbs hydrogen.

Yamamoto, H. *et al, Appl. Phys. Lett.*, 1984, **45**, 1141 (*magnetism*)
Andreev, A.V. *et al, Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)
Pinkerton, F.E. *et al, J. Appl. Phys.*, 1985, **57**, 4121 (*mössbauer*)
Duh, O.M. *et al, CA*, 1986, **105**, 201912 (*synth, cryst struct*)
Rosenberg, M. *et al, Hyperfine Interact.*, 1986, **28**, 503 (*mössbauer, struct*)
Hirosawa, H. *et al, J. Appl. Phys.*, 1986, **59**, 873 (*magnetism*)

$BFe_{14}Ho_2$ IC-000844
Holmium iron boride ($Ho_2Fe_{14}B$)
[94186-35-3]

$Ho_2Fe_{14}B$

M 1122.5
Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. Has applications in magnet technology. T_c 577K. Absorbs hydrogen.

Andreev, A.V. *et al*, *Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)
Pinkerton, F.E. *et al*, *J. Appl. Phys.*, 1985, **57**, 4121 (*mössbauer, struct*)
Dub, O.M. *et al*, *CA*, 1986, **105**, 201912 (*synth, cryst struct*)
Hirosawa, H. *et al*, *J. Appl. Phys.*, 1986, **59**, 873 (*magnetism*)

IC-000845

$BFe_{14}Nd_2$
Iron neodymium boride ($Fe_{14}Nd_2B$)
[92090-39-6]

$Nd_2Fe_{14}B$

M 1081.1
Tetragonal lattice with 4 molecules per cell. Nd atoms at centre of hexagonal prisms of B atoms, and B atoms at centres of trigonal prisms of Fe atoms. Synth. from Fe,B, B and Nd at 700-1000°, sintering at 550-650° or from elements at 1130°. High coercive strength ferromagnet, mag. props. enhanced by inclusion of small amounts of Tb, Dy, Co. Mp *ca.* 1450°. T_c 600K (581 K). Absorbs H_2.

Li, Hh, *Mater Lett.*, 1984, **2**, 453 (*cryst struct*)
Shoemaker, C.B. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 1665 (*cryst struct*)
Sinha, P. *et al*, *Scr. Metall.*, 1984, **18**, 221 (*magnetism*)
Givord, D. *et al*, *Solid State Commun.*, 1984, **50**, 497 (*cryst struct*)
Pinkerton, F. *et al*, *J. Appl. Phys.*, 1985, **57**, 2784 (*Nd-145, Nd-145 mössbauer*)
Narasimhan, K.S.V.L. *et al*, *J. Appl. Phys.*, 1985, **57**, 4081 (*cryst struct, magnetism*)
Herbst, J.F. *et al*, *J. Appl. Phys.*, 1985, **57**, 4086 (*struct, mol, cryst struct, magnetism*)
Pinkerton, F.E. *et al*, *J. Appl. Phys.*, 1985, **57**, 4121 (*mössbauer*)
Kanai, K. *et al*, *Phys. Rev. B*, 1985, **32**, 1756 (*mössbauer*)
U.S. Pat., 4,541,877, (1985); *CA*, **103**, 204696 (*use*)
Rosenberg, M. *et al*, *Hyperfine Interact.*, 1986, **28**, 503 (*mössbauer, magnetism*)
Hirosawa, H. *et al*, *J. Appl. Phys.*, 1986, **59**, 873 (*magnetism*)
Gueramian, D.E., *J. Crystal Growth*, 1986, **75**, 277 (*synth*)
Chang, Yu-Jin *et al*, *Phys. Status Solidi A*, 1986, **93**, 573 (*struct*)
Gunther, A. *et al*, *Scr. Metall.*, 1987, **21**, 607 (*use*)

$BFe_{14}Pr_2$
Iron praseodymium boride ($Fe_{14}Pr_2B$)
[93486-52-4]

$Pr_2Fe_{14}B$

M 1074.4
Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. T_c 570K (469K). Absorbs hydrogen.

Andreev, A.V. *et al*, *Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)
Herbst, J.F. *et al*, *J. Appl. Phys.*, 1985, **57**, 2343 (*mol, struct*)
Bozorth, E. *et al*, *J. Appl. Phys.*, 1985, **57**, 4106 (*magnetism*)
Pinkerton, F.E. *et al*, *J. Appl. Phys.*, 1985, **57**, 4121 (*mössbauer*)
Rosenberg, J.R.K. *et al*, *J. Appl. Phys.*, 1985, **57**, 4127 (*magnetism, mössbauer*)
Hirosawa, H. *et al*, *J. Appl. Phys.*, 1986, **59**, 873 (*magnetism*)

$BFe_{14}Sm_2$ IC-000847
Iron samarium boride ($Fe_{14}Sm_2B$)
[94186-36-4]

$Sm_2Fe_{14}B$

M 1093.3
Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. Useful in magnet technology. T_c 620K. Absorbs hydrogen.

Andreev, A.V. *et al*, *Dokl. Akad. Nauk SSSR*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)
Dub, O.M. *et al*, *CA*, 1986, **105**, 201912 (*synth, cryst struct*)
Hirosawa, H. *et al*, *J. Appl. Phys.*, 1986, **59**, 873 (*magnetism*)

$BFe_{14}Th_2$ IC-000848
Iron thorium boride ($Fe_{14}Th_2B$)
[99251-10-2]

$Th_2Fe_{14}B$

M 1256.7
Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. T_c 490K. Absorbs hydrogen.

Andreev, A.V. *et al*, *Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)

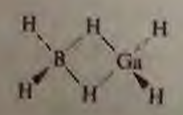
$BFe_{14}Y_2$ IC-000849
Iron yttrium boride ($Fe_{14}Y_2B$)
[93388-53-5]

$Y_2Fe_{14}B$

M 970.4
Tetragonal lattice ($Nd_2Fe_{14}B$ type struct.) with 9-coord. B. Synth. from elements. T_c 580K. Absorbs hydrogen.

Andreev, A.V. *et al*, *Dokl. Akad. Nauk SSSR (Physics Sect.)*, 1985, **283**, 1369; *Sov. Phys.-Dokl. (Engl. Transl.)*, 1985, **30**, 720 (*cryst struct, magnetism*)
Pinkerton, F.E. *et al*, *J. Appl. Phys.*, 1985, **57**, 4121 (*mössbauer, struct*)
Dub, O.M. *et al*, *CA*, 1986, **105**, 201912 (*synth, cryst struct*)
Hirosawa, H. *et al*, *J. Appl. Phys.*, 1986, **59**, 873 (*magnetism*)

$BGaH_6$ IC-000850
Gallaborane(6)



M 86.5
Colourless gas. Sol. toluene. Mp *ca.* −45°. V. p. *ca.* 1 mm at −78°. Dec. at > −35°.

Pulham, C.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1990, 177 (*synth, ir, pmr, ^{11}B nmr, ed, struct*)

[BGd] IC-000851
Gadolinium borides
[60861-13-4]

Gadolinium boride (GdB_2), 9CI, 8CI [60304-77-0]
B_2Gd M 178.8
Has the AlB_2-type struct. Synth. from Gd + B at 1240° and high pressure.

Gadolinium boride (GdB_4), 9CI, 8CI [12007-54-4]
Gadolinium tetraboride

B_4Gd M 200.4
Has the tetragonal UB_4-type struct. Synth. from Gd_2O_3 + B at 1800°; or by melting GdB_6. Golden lustrous cryst. Mp *ca.* 3000°. μ_{eff} = 8.07 (7.4)μ_B. Antiferromagnetic at low temp.

Gadolinium boride (GdB_6), 9CI, 8CI [12008-06-9]
Gadolinium hexaboride
B_6Gd M 222.1
Synth. from Gd_2O_3 + B at 1500-1850°, or from Gd_2O_3 + H_3BO_3 + Mg at 1200°. Employed in hard metal coatings. Violet cryst. Mp 2510° dec. At 1925° dissociates into elements via GdB_4 (at 1550°).

Gadolinium boride (GdB_{12}), 9CI, 8CI [37342-51-1]
Gadolinium dodecaboride
$B_{12}Gd$ M 286.9
Cubic UB_{12}-type struct. Synth. from elements at high pressure.

Gadolinium boride (GdB_{66}), 9CI [37322-40-0]
$B_{66}Gd$ M 870.7
Struct. has B_{12} icosahedron surrounded by 12 B_{12} linked icosahedra. Unit cell contains 1584 B atoms and 24 Gd atoms. Synth. from elements. Mp *ca.* 2150°. V. hard and refractory.

Manelis, R.M. *et al*, *Poroshk. Metall. (Kiev)*, 1966, **6**, 77; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1966, **6**, 904 (*synth*)
Gordienko, S.P. *et al*, *Zh. Fiz. Khim.*, 1966, **40**, 3092; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1966, **40**, 1659.
Markovskii, L.Ya. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1824; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1752 (*synth*)
Timofeeva, N.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1789; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1559 (*synth*)
Kudintseva, G.A. *et al*, *Poroshk. Metall. (Kiev)*, 1968, **8**, 45; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1968, **8**, 115 (*synth*)
Mordovin, O.A. *et al*, *Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Buschow, K.H.J. *et al*, *J. Chem. Phys.*, 1972, **57**, 3910 (*magnetism*)
Schwetz, K. *et al*, *J. Less-Common Met.*, 1972, **26**, 99 (*synth*)
Cashion, J.D. *et al*, *J. Phys. C*, 1973, **6**, 2611 (*mössbauer*)
Ames, L.L. *et al*, *High Temp. Sci.*, 1975, **7**, 44 (*ms*)
Chazalviel, J.N. *et al*, *Phys. Rev. Lett.*, 1976, **37**, 919 (*pe*)
Ishii, M. *et al*, *Solid State Commun.*, 1976, **20**, 437 (*raman*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Cannon, J.F. *et al*, *J. Less-Common Met.*, 1977, **56**, 83 (*synth*)
Etourneau, J. *et al*, *J. Less-Common Met.*, 1979, **67**, 531 (*synth, magnetism, electrical props*)
Tanaka, T. *et al*, *J. Appl. Phys.*, 1980, **51**, 3877 (*synth, purifn, electrical props*)
Golikova, O.A. *et al*, *J. Less-Common Met.*, 1981, **82**, 169 (*synth, electrical props*)

$BGeH_6^{\ominus}$ IC-000852
Germyltrihydroborate(1−)

$[H_3GeBH_3]^{\ominus}$

M 89.4 (ion)
K salt: [21349-89-3]. *Potassium germyltrihydroborate*
$BGeH_4K$ M 128.5
Moisture sensitive white solid (Et_2O). Mp 98-99° (under Ar). When heated to 200° dec. to H_2, volatile GeH_4, Ge and KBH_4.

Rustad, D.S. *et al*, *Inorg. Chem.*, 1968, **7**, 213 (*synth, ir, pmr, props*)

BHI_2 IC-000853
Diiodoborane, 10CI, 9CI
[43338-13-2]

I_2BH

M 265.6
Prototype of the alkyldiiodoborane series of compds. Prepd. *in situ* by adding I_2/THF to BH_3 at 0°. Air-sensitive. Sol. THF.

Et_3N complex: [56598-29-9]. *Hydrodiiodo(triethylamine) boron. Diiodoborane triethylamine*
$C_6H_{16}BI_3$ M 352.8
Prepd. by the reaction of I_2 with triethylamine borane. Extremely sensitive to moisture, dec. on standing. Sol. toluene.

Me_3N complex: [25741-84-8]. *Hydrodiiodo(trimethylamine) boron. Diiodoborane trimethylamine*
$C_3H_{10}BI_3$ M 310.7
Prepd. by the reaction of I_2 with trimethylamine borane. Extremely sensitive to moisture, dec. on standing. Sol. toluene.

Dimethyl sulfide complex: [28920-40-3]. (*Dimethyl sulfide*) *hydrodiiodoboron. Hydrodiiodo[thiobis[methane]]boron, 10CI*
$C_2H_7BI_2S$ M 327.7
Useful means of storing diiodoborane; hydroborates alkenes to give alkyldiiodoboranes. Moisture-sensitive liq.

Phosphine complex: [41593-72-0].
BH_4I_2P M 299.6
Sol. MeI, CH_2Cl_2; pmr δ −6.30, J_{PH} 4.18 Hz; ^{31}P nmr δ + 95, J_{PH} 424 Hz.

Lowe, J.R. *et al*, *Inorg. Chem.*, 1970, **9**, 1423 (*props*)
Brown, M.P. *et al*, *J. Chem. Soc. A*, 1970, 410 (*ir*)
Rapp, B. *et al*, *Inorg. Chem.*, 1973, **12**, 2868 (*nmr*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*nmr*)
Kinberger, K. *et al*, *Z. Naturforsch., B*, 1975, **30**, 55 (*synth*)
Ashby, E.L. *et al*, *Tetrahedron Lett.*, 1976, 3865 (*synth, use*)
Brown, H.C. *et al*, *J. Org. Chem.*, 1980, **45**, 384 (*use*)

$BHMgO_3$ IC-000854
Szaibelyite, 9CI
Ascharite (absol.), Camsellite (absol.)
[12447-04-0]

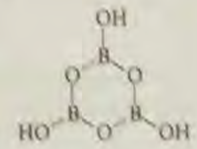
$MgBO_2(OH)$

M 84.1
Can also be formulated $2MgO.B_2O_3.H_2O$ or $Mg_2B_2O_5.H_2O$. Widespread, found in e.g. USA, Hungary, Germany, USSR, Korea, Sweden. Colourless to straw-yellow monoclinic cryst.

[36564-04-2, 51198-60-8]

Takeuchi, Y., *Mineral. J.*, 1958, **2**, 245 (*ir*)
Shamaev, P.P. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 274 (*synth*)
Takeuchi, Y. *et al*, *Am. Mineral.*, 1975, **60**, 273 (*cryst struct*)

BHO_2 IC-000855
Boric acid (HBO_2), 11CI, 10CI
Metaboric acid
[13460-50-9]



α-form (*trimer*)

M 43.8
Common product of hydrolysis and pyrolysis of many boron compds. Three cryst. forms known.

Boric acid ($H_3B_3O_6$) [13460-51-0]
α-form. HBO_2-III form. Orthorhombic-form
$B_3H_3O_6$ M 131.4
All B atoms are 3-coordinate in solid state. Colourless hygroscopic solid. Sol. H_2O. Mp 176°. ΔH_f° −788.8 kJ mol^{-1} (least stable form).

Boric acid ($H_3B_3O_7$), ***monohydrate***
β-form. HBO_2-II form. Monoclinic-form
$B_3H_5O_7$ M 149.4
Retains same skeleton as α-form, but with ¼ B additionally bonded to a water molecule. Colourless solid. Mod. sol. H_2O. Mp 200.9°. ΔH_f° −794.3 kJ mol^{-1}.

Boric acid ($H_3B_3O_8$), ***dihydrate***
γ-form. HBO_2-I form
$B_3H_7O_8$ M 167.4
Cyclic struct. of α-form is extended into 3D network of BO_4-tetrahedra with strong H-bonding in solid state. Colourless solid. Spar. sol. H_2O, alcohols. Mp 236°. ΔH_f° −804.0 kJ mol^{-1} (most stable form).

Kracek, F.C. *et al*, *Am. J. Sci.*, 1938, **35**, 143 (*B_2O_3-H_2O phase diagram, synth*)
Silver, A.H., *J. Chem. Phys.*, 1960, **32**, 959 (*B-11 nmr, α-form, β-form*)
Bray, P.J. *et al*, *J. Chem. Phys.*, 1961, **35**, 435 (*B-11 nmr, γ-form*)
Zachariasen, W.H., *Acta Crystallogr.*, 1963, **16**, 380, 385 (*cryst struct, γ-form, β-form*)
Peters, C.R. *et al*, *Acta Crystallogr.*, 1964, **17**, 229 (*cryst struct, α-form*)
Bertolozzo, A. *et al*, *J. Mol. Struct.*, 1980, **64**, 123 (*ir, raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1980, **5/A**, 224 (*rev, bibl*)

BHS IC-000856

Thioxoborane, 10Cl, 9Cl
Boron hydrogen sulfide, 8Cl
[14457-85-3]

$[BHS]_n$

M 43.8
Monomeric in gas phase at > 1200°. Polymeric in solid state. Polymer is colourless solid; readily hydrol. Insol. $CHCl_3$, C_6H_6, Et_2O, CS_2, triglyme, dioxane.

[31668-99-2]

Burg, A.B. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 3307 (*synth*)
Kirk, R.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 18 (*synth, ir, ms*)
Tanaka, J. *et al*, *J. Org. Chem.*, 1970, **35**, 1015 (*synth, ir, ms, B-11 nmr*)

BH_2I IC-000857

Iodoborane
Dihydroiodoboron

BH_2I

M 139.7

4-Methylpyridine complex: [59499-23-9]. *Dihydroiodo(4-methylpyridine)boron, 10Cl. Iodoborane γ-picoline*
C_6H_9BIN M 232.8
Identified by nmr only.

Denniston, M.L. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 379 (*synth, nmr*)
Vidal, J.L. *et al*, *Inorg. Chem.*, 1977, **16**, 1673.

$BH_2MnO_{40}W_{11}^{7\ominus}$ IC-000858

Tungstomanganoborate ($H_2BMnW_{11}O_{40}^{7\ominus}$)

$[H_2BMn^{II}W_{11}O_{40}]^{7\ominus}$

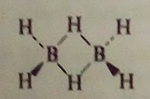
M 2730.0 (ion)
Heteropolytungstate. Rapidly formed in aq. soln. from $Mn^{2\oplus}$ and $BW_{11}O_{39}^{9\ominus}$. Free acid unstable. Solns. of $[H_2BMn^{II}W_{11}O_{40}]^{7\ominus}$ undergo oxidation in air at r.t. to give $[H_2BMn^{III}W_{11}O_{40}]^{6\ominus}$.

Hepta-K salt: Prepd. from aq. $Na_2WO_4.2H_2O$ (pH 6.3), H_3BO_3 and $Mn^{2\oplus}$ followed by addition of a K salt. Tetragonal brown yellow needles + $16H_2O$.
Na, hexa-K salt: Isol. from solns. left from the synth. of the Hepta-K salt. Solid + $14H_2O$.

Tourné, C.M., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **266**, 702, 1363 (*struct, synth, electrochem*)
Tourné, C.M. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 1124 (*synth, electrochem*)
Tourné, C.M. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 3875 (*synth, electrochem, uv-vis*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 90 (*rev, bibl*)

BH_3 IC-000859

Borane
Borine. Boron hydride
[13283-31-3]



dimer

M 13.8
Exists as the dimer (diborane) unless complexed with a nucleophilic sp. The THF soln., dimethyl sulfide complex, and other complexes are important hydroborating and reducing agents.
▷ Violent reaction with oxygen.

Dimer: [19287-45-7]. *Diborane(6), 10Cl. Boroethane*
B_2H_6 M 27.6
Hydroborating and reducing reagent as soln. in THF or ethers. Deuterated diborane useful for incorporation of deuterium into org. molecules. Thermolysis is a major route to higher boranes. Colourless air- and moisture-sensitive gas. Sol. THF as BH_3-THF complex. Mp −165.5°. Bp −92.5°.
▷ HQ9275000.

PH_3 complex: see *Trihydro(phosphine)boron, IC-000883*
Borane hydrazine complex: see *(Hydrazine-N)trihydroboron, IC-000884*
Hydrazine bis(borane) complex: see *[μ-(Hydrazine-N:N')]hexahydrodiboron, IC-000998*
$MeNH_2$ complex: see *Trihydro(methylamine)boron, IC-002627*
Methylhydrazine bis(borane) complex: see *Methylhydrazine bis(borane), IC-002655*
Isocyanomethane complex: see *Borane isocyanomethane, IC-003166*
Me_2S complex: see *(Dimethyl sulfide)trihydroboron, IC-003306*
Me_2NH complex: see *(Dimethylamine)trihydroboron, IC-003313*
Me_2PH complex: see *(Dimethylphosphine)trihydroboron, IC-003314*
Me_3N complex: see *Trihydro(trimethylamine)boron, IC-003716*

$(MeO)_3P$ complex: see *Trihydro(trimethyl phosphite-P)boron, IC-003718*
Me_3P complex: see *Trihydro(trimethylphosphine)boron, IC-003719*
THF complex: see *Trihydro(tetrahydrofuran)boron, IC-004177*
Morpholine complex: see *Trihydro(morpholine-N⁴)boron, IC-004200*
tert-Butylamine complex: see (tert-*Butylamine*) *trihydroboron, IC-004292*
Et_2NH complex: see *(Diethylamine)trihydroboron, IC-004293*
Py complex: see *Trihydro(pyridine)boron, IC-004719*
4-Aminopyridine complex: see (*4-Aminopyridine*) *trihydroboron, IC-004720*
(2-Methoxyethyl)dimethylamine complex: see *[Dimethyl(2-methoxyethyl)amine]trihydroboron, IC-004768*
4-Methylpyridine complex: see *Trihydro(4-methylpyridine) boron, IC-005073*
Et_3N complex: see *Trihydro(triethylamine)boron, IC-005300*
(2-Ethoxyethyl)dimethylamine complex: see *[(2-Ethoxyethyl) dimethylamine]trihydroboron, IC-005301*
TMED complex: see *Trihydro(N,N,N′,N′-tetramethyl-1,2-ethanediamine-N)boron, IC-005421*
TMED complex (1:2): see *Hexahydro[μ-(N,N,N′,N′-tetramethyl-1,2-ethanediamine-N:N′)]diboron, IC-005475*
Tris(dimethylamino)phosphine complex: see *(Hexamethylphosphorous triamide)trihydroboron, IC-005464*
2,6-Dimethylpyridine complex: see (*2,6-Dimethylpyridine*) *trihydroboron, IC-005748*
N,N-Dimethylaniline complex: see (N,N-*Dimethylaniline*) *trihydroboron, IC-006027*
Ephedrine complex: see (*Ephedrine*)*trihydroboron, IC-006996*
Ph_3N complex: see *Trihydro(triphenylamine)boron, IC-009881*
Ph_3P complex: see *Trihydro(triphenylphosphine)boron, IC-009882*
Monodeutero compd.: [19136-69-7].
B_2DH_5 M 28.6
Present in mixts. of B_2H_6 + B_2D_6; not isol. pure.
Dideutero compd.: [81748-50-7].
$B_2D_2H_4$ M 29.6
Present in mixt. of B_2H_6 + B_2D_6; not isol. pure.
Hexadeutero compd.: [20396-66-1].
B_2D_6 M 33.7
Colourless gas. Bp −93.4°.

Burg, A.B., *J. Am. Chem. Soc.*, 1952, **74**, 1340 (*synth, D_6 compd*)
Schlesinger, H. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 199 (*synth*)
Ditter, J.F. *et al*, *J. Phys. Chem.*, 1960, **64**, 1682 (*ms, D_6 compd*)
Bartell, L.S. *et al*, *J. Chem. Phys.*, 1965, **42**, 1135 (*ed, gas phase struct, D_6 compd*)
Allerhand, A. *et al*, *J. Chem. Phys.*, 1969, **50**, 5037 (*B-11 nmr, D_6 compd*)
Naiman, K. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 74 (*pmr*)
Solomon, J.L. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 1443 (*ms*)
Leach, J.B. *et al*, *J. Magn. Reson.*, 1972, **6**, 74 (*nmr*)
Odom, J.D. *et al*, *Inorg. Chem.*, 1973, **12**, 95 (*nmr*)
Carriera, L.A. *et al*, *J. Chem. Phys.*, 1973, **59**, 4955 (*raman, D_6 compd*)
Murano, Y. *et al*, *Radiochem. Radioanal. Lett.*, 1980, **44**, 315 (*deriv, synth*)
Leach, J.B. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 988 (*synth*)
Duncan, J.L. *et al*, *J. Mol. Spectrosc.*, 1981, **85**, 16 (*ir, D_6 compd*)
Duncan, J.L. *et al*, *Mol. Phys.*, 1984, **51**, 371 (*gas phase struct, D_6 compd*)

BH_3O IC-000860

Hydroxyborane
Borinic acid, 10Cl, 9Cl
[35825-58-2]

H_2BOH

M 29.8
Prototype member of the dialkyl(hydroxy)boranes. Unstable to moisture and to self-decomposition. Dipole moment 1.506D.

Gropen, O. *et al*, *J. Mol. Struct.*, 1975, **25**, 161 (*props*)
Hinde, A.L. *et al*, *J. Comput. Chem.*, 1980, **1**, 118 (*props*)
Kawashima, Y. *et al*, *J. Chem. Phys.*, 1981, **74**, 5430 (*microwave*)
Boggs, J.E. *et al*, *Theochem*, 1981, **1**, 329; *CA*, **95**, 103720a (*struct*)
Sliznev, V.V. *et al*, *CA*, 1982, **97**, 118997m.

BH_3O_3 IC-000861

Boric acid (H_3BO_3), 9Cl, 8Cl
Boracic acid. Orthoboric acid
[10043-35-3]

$B(OH)_3$

M 61.8
Common product of hydrol. of many boron compds. containing B—Hal, OR, SR, H, NR_2 etc. bonds. Antibacterial agent. Commercially available. Widely used in industry, e.g. precursor for borate glasses, component of buffer solns., fluxes for welding, fireproofing material. Catalyst for air oxidation of hydrocarbons and esterification of carboxylic acids. Pearly scales. Mp 171°. Component of Aci-Jel, Blinx, Bluboro, Borofax, Collyrium Eye Drops, Wyanoids. ΔH_f° −1094.3 kJ mol^{-1}. Melting point often indefinite owing to gradual dehydration on heating.
▷ ED4550000.

Mineral-form
Sassolite
Found in the waters of various lakes, eg. in Tuscany, Germany, California; also associated with hot springs. White to grey soft pearly triclinic cryst.

Zachariasen, W.H., *Acta Crystallogr.*, 1954, **7**, 305 (*cryst struct*)
Sciarra, E., *J. Am. Pharm. Assoc., Sci. Ed.*, 1960, **49**, 116 (*tox*)
Craven, B.M. *et al*, *Acta Crystallogr.*, 1966, **20**, 214 (*nd*)
Nöth, H. *et al*, *NMR Spectroscopy of Boron Compounds* (*NMR Basic Principles and Progress*, Springer Verlag, 1978 (*B-11 nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 75 (*manuf, uses*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1980, **5**, 224 (*rev, bibl*)
Butler, L.G. *et al*, *J. Magn. Reson.*, 1981, **42**, 120 (*nqr*)
Janda, R. *et al*, *Spectrochim. Acta, Part A*, 1981, **36**, 997 (*ir, raman*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 260.
Houlsby, R.D. *et al*, *Antimicrob. Agents Chemother.*, 1986, **29**, 803 (*pharmacol*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *3rd Suppl.*, 1987, **2**, 96 (*rev, bibl*)

$BH_3O_{12}S_3$ IC-000862

Boron tri(hydrogensulfate)
Sulfuric acid anhydride with boric acid (H_3BO_3) (3:1), 11Cl, 10Cl
[67374-74-7]

$B[OS(O)_2OH]_3$

M 302.0

Colourless powder, dehydrates. Sol. anhyd. H_2SO_4. Mp >240° (sealed tube).

Greenwood, N.N. *et al. J. Chem. Soc.*, 1959, 3840 (synth)
Kreshkov, A.P. *et al. Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, 23, 857 (synth, ir, thermal anal)

IC-000883

BH_4^-

Borohydride(1 –)

Tetrahydridoborate(1 –)

$[BH_4]^-$

M 14.8 (ion)

Li salt: see *Lithium borohydride*. *IC-000887*

Na salt: see *Sodium borohydride*. *IC-000888*

Dodd, T. *et al. J. Phys. Chem.*, 1959, **63**, 1555 (raer)
Jones, R. *et al. Prog. Inorg. Chem.*, 1970, **12**, 129 (synth)

IC-000884

BH_4K

Potassium borohydride

Potassium tetrahydroborate(III). Tetrahydridoborate, potassium salt, 8CI

[13762-51-0]

KBH_4

M 53.9

Synth. by reaction of B_2H_6 with $KB(OMe)_4$ in Et_2O. Commercially available. Reducing agent, extensively used in the recovery of precious metals. Moisture-sensitive white cubic cryst. Dec. on heating into constit. elements. V. sol. H_2O (19 g per 100 cm^3 at 20°); spar. sol. EtOH; MeOH; insol. Et_2O. ΔH_f° −227 kJ mol^{-1}; ΔG_f° −160 kJ mol^{-1}; S° 106.6 J K^{-1} mol^{-1}

▷ Flammable. 75752500.

Schlesinger, H.I. *et al. J. Am. Chem. Soc.*, 1953, **75**, 186 (synth)
King, A.J. *et al. J. Am. Chem. Soc.*, 1956, **78**, 4178 (cryst struct)
Volkov, V.V. *et al. Zh. Neorg. Khim.*, 1968, **13**, 659 (ir)
Bagnall, K., *Plutt. Surf.*, 1978, **59**, 29; *CA*, **89**, 178703 (rev)
Chase, M.W. *et al. J. Phys. Chem. Ref. Data*, 1985, **14**, 252 (thermochem data)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2001D (loc)

IC-000885

BH_4Li

Lithium borohydride

Lithium tetrahydroborate(III). Tetrahydridoborate(1 –), lithium salt, 8CI

[16949-15-8]

$LiBH_4$

M 21.7

Commercially available as solid or in THF solv. Prepd. by metathesis of $NaBH_4$ with lithium salts in ethereal solvs. Versatile reducing agent for aldehydes, ketones, acid chlorides, lactones, epoxides and esters.Reagent for synth. of other borates. Colourless orthorhombic cryst. Moisture sensitive. Dec. on heating with formation of constituents in elemental form. Sol. Et_2O, THF. Mp 284° (268°). Unstable >280°. ΔH_f° −190.5 kJ mol^{-1}; ΔG_f° −124.7 kJ mol^{-1}; S° 75.8 J K^{-1} mol^{-1}

▷ Flammable. Reacts violently with H_2O. OJ6427000.

Harris, P.M. *et al. J. Am. Chem. Soc.*, 1947, **69**, 1231 (cryst struct)
Gmelin Handbook Inorg. Chem., Syst. No. 20, 1980, 487 (rev, bibl)
Brown, H.C., *Hydroboration*, W.A. Benjamin, Inc., N.Y., 1962, 243 (raer)
Volkov, V.V. *et al. Zh. Neorg. Khim.*, 1968, **13**, 659 (ir)
Brown, H.C. *et al. Inorg. Chem.*, 1982, **21**, 3657 (synth)
Chase, M.W. *et al. J. Phys. Chem. Ref. Data*, 1985, **14**, 233 (thermochem data)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2101A

IC-000886

BH_4LiO_4

Lithium tetrahydroxyborate, 8CI

Lithium metaborate dihydrate. Dilithium diborate tetrahydrate

[12008-96-1]

$Li[B(OH)_4]$

M 85.7

May also be formulated $LiBO_2.2H_2O$ or $Li_2O.B_2O_3.4H_2O$. Colourless cryst. Sol. H_2O. Loses H_2O below 200°

Hexahydrate: [63454-43-5]. *Lithium tetrahydroxyborate hexahydrate, 8CI. Lithium metaborate octahydrate. Lithium diborate hexadecahydrate*

$BH_{16}LiO_{10}$ M 195.8

Colourless cryst. Sol. H_2O. Contains discrete $B(OH)_4^-$ anions, but is also formulated as $LiBO_2.8H_2O$ or $Li_2O.B_2O_3.16H_2O$. Loses $4H_2O$ at 70°, and two more between 140-280°.

Bekturs, W.T. *et al. J. Phys. Chem.*, 1955, **59**, 19 (*thermochem*)
Kuznetsov, L. *et al. Acta Crystallogr.*, 1965, **19**, 747 (*cryst struct*)
Bonhoeffer, K., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1442 (*synth, thermochem*)
Mazurek, M. *et al. Z. Anorg. Allg. Chem.*, 1972, **387**, 290 (*synth, ir, raman, thermochem*)
Zviedre, I. *et al. CA*, 1974, **80**, 140635 (*thermal anal*)
Nakamura, S. *et al. CA*, 1975, **82**, 116745 (*thermochem, thermal anal*)
Dzene, A. *et al. CA*, 1979, **90**, 145201; 1980, **93**, 196913 (*thermochem, thermal anal*)

IC-000887

BH_4N

Aminoborane, 8CI

Boranamine, 8CI. 9CI. Aminoborine

[14728-15-5]

H_2BNH_2

M 28.8

Parent system for a range of organic aminoborane derivs. Air- and moisture-sensitive gas (solid aminoborane polymerises between −196° and −155° to yield inert white material). Dipole moment 1.844D.

Schaeffer, G.W. *et al. J. Am. Chem. Soc.*, 1955, **77**, 331 (*synth*)
Kuznesof, P.M. *et al. J. Am. Chem. Soc.*, 1968, **90**, 2557 (*ms*)
McGee, H.A. *et al. Inorg. Chem.*, 1970, **9**, 2458 (*ms, ir, synth*)
Yagge, M. *et al. Chem. Phys. Lett.*, 1979, **64**, 573
Dewar, M.J.S. *et al. J. Mol. Struct.*, 1980, **68**, 105 (*ir*)
Hashlem, R.C., *Pure Appl. Chem.*, 1982, **54**, 1129

IC-000888

BH_4Na

Sodium borohydride

Tetrahydroborate, sodium salt, 8CI. Sodium tetrahydroborate(III)

[16940-66-2]

$NaBH_4$

M 37.8

Commercially available either as solid, supported on alumina or silica gel or in soln. in diglyme, triglyme or aq. sodium hydroxide. Manuf. by reaction of NaH with boron hydrides (B_2H_6) or boron trihalides (BF_3) in ethereal solvs. Versatile reducing agent. White cubic cryst. Dec. on heating into constituent elements. V. sol H_2O (56 g per 100 cm^3 at 24°); mod. sol. EtOH, MeOH

spar. sol. Py; insol. Et_2O; sol. liq. NH_3. Mp 49?°. Dissolves in cold H_2O to cryst. as the dihydrate; at higher temps. hydrolysis occurs. ΔH_f° −191.8 kJ mol^{-1}; ΔG_f° −127.1 kJ mol^{-1}; S° 101.4 J K^{-1} mol^{-1}

▷ Flammable solid, corrosive. ED3325000.

Perm-deuterio deriv.: [15681-89-7]. *Sodium borodeuteride. Sodium tetradeuteroborate*

BD_4Na M 41.8

Synth. by reaction of $Na[B(OMe)_4]$ with B_2D_6. Versatile deuterating agent. White cubic cryst. V. sol. H_2O; mod. sol. EtOH, MeOH; spar. sol. Py; insol. Et_2O; sol. liq. NH_3.

Ford, P.T. *et al. Acta Crystallogr.*, 1954, **7**, 604 (*cryst struct*)
Taylor, R.C. *et al. J. Am. Chem. Soc.*, 1958, **80**, 27 (*raman*)
Emery, A.R. *et al. J. Chem. Phys.*, 1958, **28**, 1029 ($NaBD_4$, *synth, raman*)
Clark, T.P. *et al. J. Phys. Chem.*, 1959, **63**, 1533 (*IR-II anal*)
Davies, R.E. *et al. J. Am. Chem. Soc.*, 1960, **82**, 5950 ($NaBD_4$, *hydrolysis*)
Schaeffer, C.D.Jr., *Spectrochim. Acta*, 1960, **16**, 1054 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No.21, 1964, **1**, 257, 1968, **3**, 1251 (*rev, bibl*)
Pryakhin, P., *Ann. Univ. Turku, Ser. A*, 1967, **103**, 46; *CA*, 1968, **68**, 13070 ($NaBD_4$, *D-2 anal*)
Canadian Pat., 762 843; *CA*, 1967, **67**, 116184 (*manuf, $NaBD_4$*)
Roth, R.E. *et al. Inorg. Chem.*, 1977, **16**, 2157 ($NaBD_4$, *B-11 anal*)
Buschow, W. *et al. Pure Appl. Chem.*, 1977, **49**, 723 (*rev, bibl, anal*)
Hermann, W.A. *et al. J. Am. Chem. Soc.*, 1979, **101**, 2744 (*anal, $NaBD_4$*)
Ingman, P. *et al. Inf. Chim.*, 1985, **258**, 115 (*rev*)
Evans, W.W. *et al. J. Phys. Chem. Ref. Data*, 1985, **14**, 234 (*thermochem data*)
Ouvrard, G. *et al. J. Solid State Chem.*, 1985, **59**, 393 ($NaBD_4$, *cryst struct*)
Ueno, K., *Bull. Chem. Soc. Jpn.*, 1986, **59**, 1457 (*Na-23 anal*)

IC-000889

BH_4NaO_4

Sodium tetrahydroxyborate

Sodium metaborate dihydrate

[7632-04-4]

$Na[B(OH)_4]$

M 101.8

May also be formulated as $NaBO_2.2H_2O$ or $Na_2O.B_2O_3.4H_2O$. Component in cloth finishing treatments, detergents, photographic solns. and agricultural sprays. Colourless cryst. (H_2O), loses H_2O on standing at r.t. Sol. H_2O, MeOH, spar. sol. EtOH. Reacts with CO_2.

Dihydrate: [10555-76-7]. *Sodium tetrahydroxyborate dihydrate. Disodium diborate tetrahydrate*

BH_8NaO_6 M 137.8

Colourless cryst. Dehydrates *in vacuo*.

[7398-31-6]

Abbott, H. *et al. Z. Anorg. Allg. Chem.*, 1943, **251**, 167 (*synth*)
Xie, J., *Anal. Chem.*, 1951, **23**, 806 (*struct*)
Block, S. *et al. Acta Crystallogr.*, 1963, **16**, 1233 (*cryst struct, dihydrate*)
Kessler, G. *et al. Z. Anorg. Allg. Chem.*, 1965, **338**, 179 (*ir, dihydrate*)
Nee, N.P. *et al. J. Chem. Eng. Data*, 1967, **12**, 303 (*synth, dihydrate*)
Tramano, P. *et al. Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **271**, 1577 (*thermal anal*)
Ulrich, R. *et al. Z. Naturforsch., B*, 1979, **34**, 585 (*raman*)
Ulrich, R. *et al. Spectrochim. Acta, Part A*, 1980, **36**, 997 (*ir, raman*)

IC-000890

$BH_4O^\ominus$

Trihydroxidohydroxyborate(1 –), 10CI, 9CI, 8CI

[34492-48-6]

$[HO(BH_2)_3]^\ominus$

M 30.8 (ion)

Intermed. in hydrol. of tetrahydroborate anion.

Li salt: [81717-91-0].
BH_4LiO M 37.7
Reducing agent.

Na salt: [16940-22-9].
BH_4NaO M 53.8

K salt: [83706-85-4].
BH_4KO M 69.9
Reducing agent.

Wang, P.T. *et al. Inorg. Chem.*, 1972, **11**, 1081 (*prep*)
Reed, J.W. *et al. J. Am. Chem. Soc.*, 1974, **96**, 1248 (*synth*)
Srivastava, O. *et al. Acta Chem. Scand., Ser. A*, 1977, **31**, 385 (*prep*)
Reed, J.W. *et al. J. Org. Chem.*, 1977, **42**, 3763 (*raer*)
Reed, J., *CA*, 1978, **89**, 43401x (*synth, prep*)

IC-000871

$BH_4O_4^\ominus$

Tetrahydroxyborate(1 –), 8CI

[13840-83-7]

$[B(OH)_4]^\ominus$

M 78.8 (ion)

Conjugate base of Boric acid (H_3BO_3). *IC-000886*.

Li salt: see *Lithium tetrahydroxyborate*. *IC-000886*

Na salt: see *Sodium tetrahydroxyborate*. *IC-000889*

Ba salt: see *Barium tetrahydroxyborate*. *IC-000844*

Gmelin Handbook Inorg. Chem., Syst. No. 13, 1st Suppl., 1977, 207 (*rev, bibl*)
Nöth, H. *et al.*, *NMR Spectroscopy of Boron Compounds*, 1983, *Basic Principles and Progress, Springer-Verlag*, 1978, **31**, 1 (*rev*)
Janda, R. *et al. Z. Naturforsch., B*, 1979, **34**, 707 (*ir, synth*)
Effenberger, H., *Acta Crystallogr., Sect. B*, 1982, **38**, 1 (*cryst struct*)
Volokhov, Yu.A. *et al. CA*, 1983, **98**, 58686 (*ir, raman, anal, B-11 anal*)

IC-000872

BH_4Rb

Rubidium borohydride

Rubidium tetrahydroborate(III). Tetrahydridoborate(1 –), rubidium salt, 8CI

[20346-89-4]

$RbBH_4$

M 100.3

NaCl struct. Prepd. by reaction of $NaBH_4$ with RbOH in aq. EtOH. Colourless cubic cryst. V. sol. H_2O.

Abrahams, S.C. *et al. J. Chem. Phys.*, 1954, **22**, 434 (*cryst struct*)
Mikheeva, V.I. *et al. Zh. Neorg. Khim.*, 1966, **11**, 1506 (*synth*)
Arkhipov, S.M., *Metody Poluch. Khim. Reakt. Prep.*, 1967, **17**, 81; *CA*, 1968, **69**, 58589 (*synth*)
Volkov, V.V. *et al. Zh. Neorg. Khim.*, 1968, **13**, 659 (*ir*)

IC-000873

$BH_4S^\ominus$

Trihydromercaptoborate(1 –), 8CI

$[H_3BSH]^\ominus$

M 46.9 (ion)

Li salt: [18785-98-3].
BH_4LiS M 53.8
Colourless solid. Sol. THF

Et_4N salt: [25609-09-0].
Colourless solid, dec. in moist air. Sol. liq. H_2S.

Nöth, H. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **311**, 241 (*synth*)
Spielvogel, B.F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 765 (*synth, B-11 nmr*)
Keller, P.C., *Inorg. Chem.*, 1969, **8**, 1695 (*synth, ir, B-11 nmr*)

IC-000874

$BH_4S_2^{\ominus}$

Dihydrodimercaptoborate(1 –), 8CI
(Dihydrothio)dihydroborate(1 –)

$[H_2B(SH)_2]^{\ominus}$

M 78.9 (ion)
Li salt: [18786-07-7].
BH_4LiS_2 M 85.9
Not isol. from soln.

Spielvogel, B.F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 765 (*synth, B-11 nmr*)

IC-000875

BH_4Tl

Thallium(*I*) borohydride, ($Tl(BH_4)$)
Thallium(1) tetrahydroborate

$Tl[BH_4]$

M 219.2
Ionic compd. Synth. from KBH_4 + aq. $TlNO_3$, Tl^I compds. + $LiBH_4$. White solid, dec. at 40° to give diborane and TlH. Insol. H_2O (slow dec.).

▷ Highly toxic.

Waddington, T.C., *J. Chem. Soc.*, 1958, 4783 (*synth, struct*)
Mochalov, K.N. *et al*, *Tr. Kazan. Khim.-Tekhnol. Inst.*, 1962, **30**, 282 (*nmr*)
James, B.D., *Prog. Inorg. Chem.*, 1970, **11**, 99 (*rev*)
Wiberg, E. *et al*, *Hydrides of the Elements of the Main Groups I-IV*, Elsevier, Amsterdam, 1971.

IC-000876

$BH_5Mo_6O_{40}W_6$

Molybdotungstoboric acid, 8CI
[11092-73-2]

$H_5[BMo_6W_6O_{40}]$

M 2334.5
Heteropolyacid with Keggin struct. Yellow octahedral cryst. + H_2O. Sol. H_2O.

Polotebnova, N.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1971, **16**, 1350 (*synth, str*)

IC-000877

BH_5N_2

Diaminoborane, 8CI
Boranediamine, 10CI
[18447-53-5]

$HB(NH_2)_2$

M 43.8
Parent compd. for the series of alkyldiaminoboranes. Vapour can be kept for several days at r.t. but liq. decs. to form glassy solid with evolution of NH_3.

Baird, N.C. *et al*, *Can. J. Chem.*, 1967, **45**, 2059 (*props*)
Briggs, T.S. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 7762 (*synth, nmr, ir*)
Fjeldberg, T. *et al*, *Acta Chem. Scand., Ser. A*, 1980, **34**, 547 (*props, struct*)
Thorne, L.R., *CA*, 1980, **92**, 138026u (*ir, struct*)
Briggs, T.S., *CA*, 1981, **94**, 163335t (*props*)

IC-000878

$BH_5O_{16}S_4$

Hydrogen tetrakis(hydrogensulfato)borate, 8CI
Tetrakis(bisulfato)boric acid. Tetra(hydrogen sulfato)boric acid
[16949-98-7]

$HB[OS(O)_2OH]_4$

M 400.1
Stronger acid than HSO_3F. Moist solid at r.t., indefinite Mp, dec. on heating.

Flowers, R.H. *et al*, *J. Chem. Soc.*, 1956, 1925 (*synth*)
Gillespie, R.J. *et al*, *Can. J. Chem.*, 1960, **38**, 1371; 1962, **40**, 784 (*pmr, raman*)
Barr, J. *et al*, *Can. J. Chem.*, 1961, **39**, 1266 (*synth*)
Gillespie, R.J. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5083 (*synth*)

IC-000879

$BH_5O_{40}W_{12}$

Tungstoboric acid ($H_5BW_{12}O_{40}$), 9CI
12-Tungstoboric acid, 8CI. 12-Borotungstic acid
[12297-12-0]

$H_5[BW_{12}O_{40}]$

M 2862.0
Heteropolyanion with α-Keggin struct. (see Tungstosilicate ($SiW_{12}O_{40}^{4\ominus}$), IC-021712 for a description). Cryst. Sol. H_2O. Exists in a number of hydrated forms.

Varfolomeev, M.B. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **472**, 185 (*thermal anal, ir*)
Acerete, R. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 5384 (*uv, W-183 nmr*)
Chuvaev, V.F. *et al*, *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1982, **8**, 918 (*synth, pmr*)
Pope, M.T. *et al*, *Heteropoly and Isopoly Oxometalates*, Springer-Verlag, 1983 (*rev, bibl*)

IC-000880

$BH_5P^{\ominus}$

Trihydrophosphinoborate(1 –), 8CI
Phosphinotrihydroborate(1 –)

$[H_3B{-}PH_2]^{\ominus}$

M 46.8 (ion)
Li salt: [34390-49-3].
BH_5LiP M 53.7
V. moisture sensitive colourless cryst. V. sol. aprotic solvs. e.g. Et_2O, MeCN. Begins dec. at 85° *in vacuo*.

Mayer, E., *Inorg. Chem.*, 1971, **10**, 2259 (*synth, ir, raman, pmr*)

IC-000881

BH_6N

Amminetrihydroboron, 10CI
Borane monoammoniate, 8CI. Borane compound with ammonia. Ammonia borane. Borane ammoniate
[13774-81-7]

$H_3N{-}BH_3$

M 30.8
Prepd. from B_2H_6 + NH_3 in org. solvs. Also by reaction of $(NH_4)_2CO_3$ + $NaBH_4$ in THF. Reducing agent for aldehydes and ketones. Air-stable white cryst. Sol. H_2O, MeOH; mod. sol. THF, Et_2O, $CHCl_3$, EtOAc. Mp 112-114° dec.

▷ May explode when heated.

Shore, S.G. *et al*, *Inorg. Chem.*, 1964, **3**, 914 (*synth*)
Smith, J. *et al*, *J. Mol. Spectrosc.*, 1973, **45**, 327 (*ir, matrix-isol*)
Noeth, H. *et al*, *Chem. Ber.*, 1974, **107**, 3070 (*B-11 nmr, N-14 nmr*)
Hu, M.G. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 2147 (*synth*)
Andrews, G.C. *et al*, *Tetrahedron Lett.*, 1980, **21**, 693, 697 (*use*)

Hoon, C.F. *et al*, *J. Phys. C*, 1983, **16**, 6129 (*cryst struct*)
Wrackmeyer, B. *et al*, *J. Magn. Reson.*, 1986, **66**, 172 (*N-15 nmr*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 543.

IC-000882

BH_6N_3

Boron amide ($B(NH_2)_3$)
Boranetriamine, 9CI. Boramide
[14939-14-1]

$B(NH_2)_3$

M 58.8
Not obt. in a pure state. Formed by the action of NH_3 on BCl_3. Gas. On heating gives borimide, $B_2(NH)_3$.

Joannis, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1902, **135**, 1106 (*synth*)
Gunderssen, G., *Acta Chem. Scand., Ser. A*, 1981, **35**, 729 (*theory*)

IC-000883

BH_6P

Trihydro(phosphine)boron, 10CI
Phosphine borane (1:1), 9CI. Borane phosphine. Phosphine compd. with borane (1:1), 9CI, 8CI. Borane compd. with PH_3
[19121-56-3]

$H_3P{-}BH_3$

M 47.8
Interatomic distances (vap.): B—H 121.2, P—H 139.9, P—B 193.7 pm; angles: BPH 116.9°, PBH 103.6°, HBH 114.6°, HPH 101.3°: White solid; dissociates at r.t. Mp 32-33°. PH_3 displaceable by Me_3N.

[15120-00-0]
Rudolph, R.W. *et al*, *Inorg. Chem.*, 1966, **5**, 723 (*synth, ir, raman, pmr, B-11 nmr*)
Drake, J.E. *et al*, *J. Chem. Soc. A*, 1968, 974; 1970, 2959 (*synth, reactions*)
Cowley, A.H. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 6815 (*pmr, B-11 nmr, P-31 nmr*)
Mayer, E., *Monatsh. Chem.*, 1971, **102**, 940 (*synth*)
Rapp, B., *Inorg. Chem.*, 1973, **12**, 2868 (*nmr*)
Durig, J.R. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 2491 (*microwave, struct*)
Odom, J.D. *et al*, *J. Mol. Struct.*, 1975, **24**, 139 (*ir, raman*)
Umeyama, H. *et al*, *Chem. Pharm. Bull.*, 1981, **29**, 287 (*struct*)
Cowley, A.H. *et al*, *Inorg. Chem.*, 1982, **21**, 85 (*pe*)
Sebestyen, A. *et al*, *Theochem*, 1982, **6**, 259 (*struct*)

IC-000884

BH_7N_2

(Hydrazine-*N*)trihydroboron, 10CI, 9CI
Borane compd. with hydrazine, 9CI. Hydrazine compd. with borane, 9CI, 8CI. Borane hydrazine
[14931-40-9]

$H_2NNH_2{-}BH_3$

M 45.8
Previously considered as rocket fuel. Large translucent cryst. Mp 61° (difficult to reproduce). Dec. > 50°.

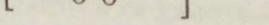
▷ Shock sensitive, nonflammable shielding necessary in synth.

Gunderloy, F.C., *Inorg. Chem.*, 1963, **2**, 221 (*synth*)
Hermanek, S. *et al*, *Collect. Czech. Chem. Commun.*, 1966, **31**, 1281 (*chromatog*)
Inorg. Synth., 1967, **9**, 13 (*synth*)
Andrianov, L.O. *et al*, *Zh. Strukt. Khim.*, 1967, **8**, 303 (*struct*)
Zakharov, V.V. *et al*, *Zh. Fiz. Khim.*, 1974, **48**, 492.
Lagodzinskaya, G.V. *et al*, *Zh. Fiz. Khim.*, 1975, **49**, 2238; 2624 (*nmr*)

IC-000885

$BH_8Na_2O_7$

Sodium perborate tetrahydrate
Sodium peroxoborate. Boric acid (HBO_2) sodium salt compd. with hydrogen peroxide (H_2O_2) (1:1) trihydrate, 8CI
[18283-88-0]



M 176.8
Generally formulated as $NaBO_2.H_2O_2.3H_2O$ although $NaBO_3.4H_2O$ was also used in the early literature. Structural analysis suggests the formulation shown above. Manuf. by electrolysis from $Na_2B_4O_7$. Chemically produced in aq. soln. from $NaBO_2$ (or $Na_2B_4O_7$ and NaOH) by reaction with either H_2O_2 or a mixture of H_2O_2 and Na_2O_2. Commercially available. Bleaching agent (containing 10.4% active oxygen); used extensively in detergents. Bactericide. Oxidising agent in org. chem. Colourless cryst. stable when cool and dry. Sol. $H_2O \rightarrow H_2O_2$. Mp 65.5° (63°). Other degrees of hydration also known.

▷ Toxic by ingestion.

[10486-00-7]
Onak, T.P. *et al*, *J. Phys. Chem.*, 1959, **63**, 1533 (*B-11 nmr*)
Miller, F.A. *et al*, *Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Hansson, A., *Acta Chem. Scand.*, 1961, **15**, 934 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 385; 1966, **3**, 1297 (*rev, bibl*)

IC-000886

[BHf]

Hafnium borides
[12653-64-4]

Hafnium boride* (*HfB*), *9CI, 8CI [12228-27-2]
Hafnium monoboride
BHf M 189.3
Observed only in ternary systems, and exists only when stabilised. Has the orthorhombic FeB-type struct. Mp 2100° dec.

Hafnium boride* (*HfB_2*), *9CI, 8CI [12007-23-7]
Hafnium diboride
B_2Hf M 200.1
Possesses the AlB_2-type struct. Synth. from elements. Strong refractory when sintered. Mp 3315° (3240°). Dissolves completely only in conc. H_2SO_4 + K_2SO_4 or $K_2S_2O_8$ at the Bp. Unreactive to H_2SO_4 + K_2SO_4 or H_3PO_4 at r.t. Reactive to conc. HCl, conc. HNO_3 mixt. or acids contg. H_2O_2.

Halleck, H., *J. Nucl. Mater.*, 1967, **21**, 14 (*synth*)
Peshev, P. *et al*, *J. Less-Common Met.*, 1968, **14**, 23 (*synth, cryst struct, props, bibl*)
Wiley, D.E. *et al*, *J. Less-Common Met.*, 1969, **18**, 149 (*props*)
Jacobs, C.G. *et al*, *Phys. Rev. B*, 1970, **1**, 839 (*mössbauer*)
Portnoi, K.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 1987; *Inorg. Materials* (*Engl. Transl.*), 1971, **7**, 1769 (*synth, phase diagram*)
Kugai, L.N. *et al*, *Poroshk. Metall.* (*Kiev*), 1971, **11**, 51; *Sov. Powder Metall. Met. Ceram.* (*Engl. Transl.*), 1971, **10**, 212 (*props*)
Jangg, G. *et al*, *Monatsh. Chem.*, 1973, **104**, 226 (*synth*)
Mavel, G. *et al*, *Surf. Sci.*, 1973, **35**, 109 (*pe*)
Voitovich, R.F. *et al*, *Poroshk. Metall.* (*Kiev*), 1975, **14**, 70; *Sov. Powder Metall. Met. Ceram.* (*Engl. Transl.*), 1975, **14**, 231 (*props*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

[BHo] – $BI_{14}Zr_6^{\ominus}$

Golovko, E.I. *et al, Poroshk. Metall. (Kiev)*, 1978, **17**, 77; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1978, **17**, 798 (*props*)

IC-000887

[BHo]

Holmium borides

***Holmium boride* (HoB_2)** [51311-01-4]

B_2Ho M 186.5

Has the hexagonal AlB_2-type struct.

Holmium boride* (HoB_4), *9CI, 8CI [12045-77-1]

Holmium tetraboride

B_4Ho M 208.1

UB_4-type struct. Black metallic cryst. Sublimes *in vacuo* without dec. Antiferromagnetic at low temp., μ_{at} = 10.4 (9.9)μ_B.

Holmium boride* (HoB_6), *9CI, 8CI [12046-36-5]

Holmium hexaboride

B_6Ho M 229.7

Cubic CaB_6-type struct. Synth. from Ho_2O_3 + B at 1500-1800° or Ho_2O_3 + B_2O_3 + Mg at 1200°. Blue solid. Mp 2180°.

***Holmium boride* (HoB_{12})**

Holmium dodecaboride

$B_{12}Ho$ M 294.6

UB_{12}-type cubic struct. Synth. from Ho_2O_3 + B at 1400-1600°. Resists HCl or H_2SO_4, and dec. only by oxidising acids.

Holmium boride* (HoB_{66}), *9CI [11141-34-7]

$B_{66}Ho$ M 878.4

Struct. contains B_{12} icosahedron surrounded by 12 B_{12} linked icosahedra. Unit cell contains 1584 B atoms and 24 Ho atoms. Synth. from elements. Mp *ca.* 2150°. V. hard and refractory.

Mordovin, O.A. *et al, Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Buschow, K.H.J. *et al, J. Chem. Phys.*, 1972, **57**, 3910 (*magnetism*)
Schwetz, K. *et al, J. Less-Common Met.*, 1972, **26**, 99 (*synth, cryst struct*)
Fisk, Z. *et al, Mater. Res. Bull.*, 1972, **7**, 285 (*synth, cryst struct*)
Ames, L.L. *et al, High Temp. Sci.*, 1975, **7**, 44 (*ms*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Cannon, J.F. *et al, J. Less-Common Met.*, 1977, **56**, 83 (*synth, cryst struct*)
Etourneau, J. *et al, J. Less-Common Met.*, 1979, **67**, 531 (*magnetic, electrical props*)
Gianduzzo, J.C. *et al, J. Less-Common Met.*, 1981, **82**, 29 (*magnetic, electrical props*)
Odintsov, V.V. *et al, Poroshk. Metall. (Kiev)*, 1984, **23**, 71; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1984, **23**, 68 (*props*)

BI_3

IC-000888

Triiodoborane, 11CI, 10CI, 9CI

Boron iodide (BI_3), 8CI. Boron triiodide

[13517-10-7]

BI_3

M 391.5

Strong Lewis acid, reacts with protic solvs. Commercially available. Colourless cryst.; light sensitive, dec. products incl. I_2. Sol. C_6H_6, CS_2, CH_2Cl_2. Mp 49.9°. Subl.$_{0.5}$ 60°, 210° (est.). ΔH_{fc}° −38.5 kJ mol^{-1}.

▷ Reacts violently with H_2O.

Lappert, M.F. *et al, J. Chem. Soc.*, 1968, 3105 (*ms*)
Bassett, P.J. *et al, J. Chem. Soc. A*, 1971, 1551 (*pe*)
Lappert, M.F. *et al, J. Chem. Soc. A*, 1971, 2426 (*B-11 nmr*)
Clark, R.J.H. *et al, J. Chem. Phys.*, 1972, **56**, 2225 (*ir, raman*)
Maria, H.J. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1050 (*uv*)
Kakubari, H. *et al, Bull. Chem. Soc. Jpn.*, 1974, **47**, 2337 (*ed, gas phase struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 801 (*synth*)
Okuda, T. *et al, Bull. Chem. Soc. Jpn.*, 1977, **50**, 1007 (*mgnr*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, 1978, **19**, 207 (*rev, bibl*)

$BI_4^{\ominus}$

IC-000889

Tetraiodoborate(1−), 11CI, 10CI, 9CI, 8CI

[36500-80-8]

$[BI_4]^{\ominus}$

M 518.4 (ion)

Et_4N salt: [23289-77-2].

V. hygroscopic colourless solid. Insol. C_6H_6, Et_2O, CCl_4, pentane. Light sensitive.

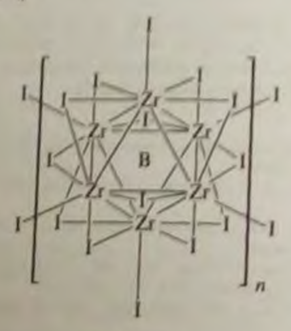
Waddington, T.C. *et al, Proc. Chem. Soc., London*, 1960, 315 (*synth, ir*)
Thompson, R.J. *et al, Inorg. Chem.*, 1965, **4**, 1464 (*B-11 nmr*)
Ahmed, I.Y. *et al, Inorg. Chem.*, 1969, **8**, 1411 (*synth, ir*)
Sheikh, S.U., *J. Therm. Anal.*, 1980, **18**, 299 (*thermal anal*)

$BI_{12}Zr_6$

IC-000890

μ_6-Borylidynedodeca-μ-iodohexazirconium, 11CI

[101054-41-5]



core cluster

M 2081.0

See also μ_6-Borylidynedodeca-μ-iododiiodohexazirconate(1−), IC-000891. Struct. attained by extensive I-bridging between clusters. Synth. by heating stoichiometric quantities of ZrI_4, Zr and B in a sealed tantalum capsule for 2 weeks at 850°. Black solid.

Smith, J.D. *et al, J. Am. Chem. Soc.*, 1986, **108**, 1927 (*synth, cryst struct*)

$BI_{14}Zr_6^{\ominus}$

IC-000891

μ_6-Borylidynedodeca-μ-iododiiodohexazirconate(1−), 11CI

As μ_6-Borylidynedodeca-μ-chlorotrichlorohexazirconate(2−), IC-000814 with

n = 1, X = I

M 2334.8 (ion)

Stoichiometry attained by extensive bridging between clusters. Synth. by heating stoichiometric quantities of ZrI_4, Zr, B and CsI(KI) in a sealed tantalum capsule for 2 weeks at 850°. Of interest because of the unusual bonding. Attempts to prepare a sodium salt result in μ_6-Borylidynedodeca-μ-iodohexazirconium, IC-000890 and unreacted NaI.

K salt: [101054-42-6].
$BI_{14}KZr_6$ M 2373.9
Black cryst.
Cs salt: [101054-43-7].
Black cryst

Smith, J.D. *et al, J. Am. Chem. Soc.*, 1986, **108**, 1927 (*synth, cryst struct*)

IC-000892

[BLa]

Lanthanum borides

[36127-33-4]

LaB_{12} appears to be unknown. Does not form LaB_{66}. LaB_y also known.

Lanthanum boride* (LaB_4), *9CI, 8CI [12007-73-7]

Lanthanum tetraboride

B_4La M 182.1

Tetragonal UB_4-type struct. Black, metal-like cryst. Mp 1800° dec. Dec. at 1800° → LaB_6 + La.

Lanthanum boride* (LaB_6), *9CI, 8CI [12008-21-8]

Lanthanum hexaboride

B_6La M 203.7

Cubic CaB_6-type struct. Synth. from La_2O_3 + B at 1500-1800° or La_2O_3 + H_3BO_3 + Mg at 1300°. Employed in optical fibres, and as high intensity electron source. Purple-pink cryst. Mp 2715° (2210°). Stable to H_2SO_4, HCl, and 40% aq. NaOH. Attacked by HNO_3. Stable to 650-700°, but ignites at 750°. Attacked by H_2O at 300° under pressure.

Johnson, R.W. *et al, J. Phys. Chem.*, 1961, **65**, 909 (*synth, phase diagram, props*)
Meerson, G.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 802; *Inorg. Materials (Engl. Transl.)*, 1967, **3**, 717 (*manuf*)
Mamedov, F.G. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 950; *Inorg. Materials (Engl. Transl.)*, 1967, **3**, 851 (*synth*)
Derenovskii, M.V. *et al, Poroshk. Metall. (Kiev)*, 1967, **7**, 8; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1967, **7**, 93 (*manuf*)
Zhuraviev, N.N. *et al, Poroshk. Metall. (Kiev)*, 1967, **7**, 95; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1967, **7**, 158 (*cryst struct*)
Markovskii, L.Ya. *et al, Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1824; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1752 (*synth*)
Timofeeva, N.I. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1789; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1559 (*synth*)
Deacon, J.A. *et al, J. Mater. Sci.*, 1971, **6**, 309 (*props, phase diagram*)
Kato, K., *Acta Crystallogr., Sect. B*, 1974, **30**, 2933 (*cryst struct*)
Ames, L.L. *et al, High Temp. Sci.*, 1975, **7**, 44 (*ms*)
Tanaka, T. *et al, J. Crystal Growth*, 1975, **30**, 193 (*purifn*)
Chazalviel, J.N. *et al, Phys. Rev. Lett.*, 1976, **37**, 919 (*pe*)
Ishii, M. *et al, Solid State Commun.*, 1976, **20**, 437 (*raman*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Aono, M. *et al, J. Phys. Chem. Solids*, 1979, **40**, 797 (*B-11 nmr*)
Noack, M.A. *et al, J. Crystal Growth*, 1980, **49**, 595 (*anal*)
Paderno, Yu.B. *et al, Poroshk. Metall. (Kiev)*, 1981, **20**, 60; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1981, **20**, 717 (*purifn*)
Korsukova, M.M. *et al, Curr. Top. Mater. Sci.*, 1984, **11**, 389 (*rev*)
Etourneau, J., *J. Less-Common Met.*, 1985, **110**, 267 (*synth*)
Hohn, F.J., *Scanning Electron Microsc.*, 1985, 1327 (*rev*)
Korsukova, M.M. *et al, J. Less-Common Met.*, 1986, **117**, 83 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1990, **C11a**, 23, 162 (*rev*)

[BLi]

Lithium borides IC-000893

LiB, LiB_4, Li_2B, Li_3B, Li_4B, Li_5B_4, Li_6B, and Li_7B_6 phases reported.

***Lithium boride* (Li_3B)** [66472-94-8]

Trilithium boride

BLi_3 M 31.6

Existence in doubt.

***Lithium boride* (LiB)** [12523-56-7]

Lithium monoboride

BLi M 17.7

Tetragonal lattice. Synth. from B + Li mixt. heated *in vacuo*. Brown solid. Mp >900° dec. When heated in inert atm., dark brown solid becomes green; change more rapid in air.

▷ Spontaneously flammable on addition of H_2O.

Sorokin, V.P. *et al, Zh. Neorg. Khim.*, 1977, **22**, 595; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 329 (*synth, props, cryst struct*)
Mitchell, M.A. *et al, J. Less-Common Met.*, 1978, **57**, 161

$BLiMnO_3$

IC-000894

Lithium manganese borate ($LiMn(BO_3)$)

$LiMnBO_3$

M 120.6

Prepared by fusing MnO and $LiBO_2$ at 1000° under N_2. Pale pink cryst.

Lehmann, H.-A. *et al, Z. Anorg. Allg. Chem.*, 1966, **348**, 49 (*synth, ir*)
Bondareva, O.S. *et al, Sov. Phys. Crystallogr. (Engl. Transl.)*, 1978, **23**, 269; 1980, **25**, 545 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 78 (*rev, bibl*)

$BLiO_2$

IC-000895

Lithium metaborate

Boric acid, lithium salt, 8CI

[13453-69-5]

$LiBO_2$

M 49.7

Prepd. by thermal treatment of an equimolar mixture of Li_2O and B_2O_3. Commercially available. Flux in x-ray fluorescence analysis. White monoclinic cryst. Mod. sol. H_2O (2.6 g per 100 cm^3 at 20°; 12 g per 100 cm^3 at 80°). Mp 844°. ΔH_f° −1019.2 kJ mol^{-1}; ΔG_f° −963.1 kJ mol^{-1}; S° 51.7 J K^{-1} mol^{-1}.

Octahydrate:

$BH_{16}LiO_{10}$ M 193.8

Prepared by aq. extraction of a previously heated mixture of Li_2CO_3 and H_3BO_3. Colourless trigonal cryst.

Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 490 (*rev, bibl*)
Hildenbrand, D.L. *et al, J. Chem. Phys.*, 1963, **39**, 296 (*synth*)
Zachariasen, W.H., *Acta Crystallogr.*, 1964, **17**, 749 (*cryst struct, octahydrate, anhydr*)
Natarajan, M. *et al, Proc. Int. Conf. Raman Spectrosc., 6th, 1978*, 1978, **2**, 354; *CA*, 1980, **92**, 206485 (*raman*)
Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 242 (*thermochem data*)

[BLu]

IC-000896

Lutetium borides

***Lutetium boride* (LuB_4)** [12688-52-7]

B_4Lu M 218.2

Black metallic cryst. Mp 255°. Diamagnetic.

Lutetium boride* (LuB_{12}), *9CI, 8CI [12589-38-7]

Lutetium dodecaboride

$B_{12}Lu$ M 304.6

UB_{12}-type cubic struct. with Lu(III) oxid. state. Synth from Lu_2O_3 + B_2O_3 + Mg at 1200°. LuB_{12}, LuB_6 and LuB_{66} have also been reported.

[12040-27-6, 60304-79-2]

Mordovin, O.A. *et al., Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Yukhimenko, E.V. *et al., Porokh. Metall. (Kiev)*, 1971, **11**, 32; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 895 (*props*)
Schwetz, K. *et al., J. Less-Common Met.*, 1972, **26**, 99
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Odintsov, V.V. *et al., Porokh. Metall. (Kiev)*, 1984, **23**, 71; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1984, **23**, 68 (*props*)
Iga, F. *et al., Solid State Commun.*, 1984, **50**, 903 (*pe*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1990, **C11a**, 6, 21; **C11b** (*rev*)

[BMg] IC-000897

Magnesium borides

[12795-15-2]

Mg borides are generally not well-characterised. There is no evidence as yet for MgB and little for MgB_4.

Magnesium boride* (MgB_2), *9CI, 8CI [12007-25-9]

B_2Mg M 45.9

AlB_2-type struct. Synth. from elements at 1200-1400°. Highly reactive to HNO_3, H_3PO_4, HCl and H_2SO_4. At 1150° → MgB_4.

***Magnesium boride* (MgB_6)** [12008-22-9]

Magnesium hexaboride

B_6Mg M 89.1

Synth. from B + Mg at 1100°. Mp 1100° dec. Resistant to boiling 6*M* HCl. Slowly attacked by boiling $HClO_4$ or conc. HNO_3, or aqua regia.

Magnesium boride* (MgB_{12}), *9CI, 8CI [12230-32-9]

Magnesium dodecaboride

$B_{12}Mg$ M 154.0

Synth. from Mg + B → MgB_7 at 1250°. Mp 1300° dec. Resistant to boiling 6*M* HCl.

[52357-03-5]

Jones, M.E. *et al., J. Am. Chem. Soc.*, 1954, **76**, 1434 (*cryst*)
Dubois, P. *Ann. Chim. (Paris)*, 1962, **7**, 339 (*synth, props*)
Ger. Pat., 1 229 505, (1966); *CA*, **66**, 47914 (*manuf*)
Gorshkalov, M.S. *et al., Zh. Prikl. Khim. (Leningrad)*, 1966, **39**, 1861; *J. Appl. Chem. USSR (Engl. Transl.)*, 1966, **39**, 1821 (*synth*)
Vedula, R. *et al., J. Solid State Chem.*, 1973, **8**, 69 (*synth, cryst struct*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev*)
Lyubimenko, V.T. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1985, **21**, 1135; *Inorg. Materials (Engl. Transl.)*, 1985, **21**, 985 (*props*)

[BMn] IC-000898

Manganese borides

Six phases described here.

Manganese boride* (Mn_4B), *10CI [12260-22-9]

BMn_4 M 230.5

Struct. built up of parallel sheets of Mn tetrahedra with B atoms in square antiprismatic voids randomly half-filled at the composition Mn_4B. Struct. may be regarded as one of Mn_3B with lower symmetry and unoccupied B places. Synth. by sintering and annealing a mixture of the elements at 1050° in sintered alumina crucibles under Ar. If temps. exceed 1100° the presence of excess B causes formation of Mn_2B and Mn. Cryst.

Manganese boride* (Mn_2B), *11CI [12045-16-8]

BMn_2 M 120.6

Struct. consists of layers of Mn atoms in close contact with isolated B atoms in square antiprismatic holes. Adopts $CuAl_2$ struct. with tetragonal symmetry. Obt. by sintering and annealing Mn-B mixtures in evacuated silica tubes at 1100-1200° for 7-10 d or in alumina crucibles under Ar at 900-1350°. Reddish brown cryst.; hard and brittle. Mp 1580°.

Manganese boride* (*MnB*), *11CI [12045-15-7]

BMn M 65.7

Struct. consists of trigonal prisms of Mn, with zig-zag chains of B (like FeB). Obt. from elements in sealed silica tubes at 1100-1200°. Lustrous reddish-brown cryst. Mp 1860-1920°. Curie temp. 578K. Ferromagnetic.

Manganese boride* (Mn_3B_4), *11CI [12229-02-6]

B_4Mn_3 M 208.0

Isostructural with Ta_3B_4, comprising trigonal prisms of Mn atoms containing one B atom or B—B double chains consisting of planar six membered rings plus Mn atoms. Synth. from the elements in evacuated silica tubes at 1100-1200° for 7-10 d. Reddish brown cryst. with a metallic lustre. Mp 1750° dec. Antiferromagnetic >230K.

Manganese boride* (MnB_2), *11CI [12228-50-1]

B_2Mn M 76.5

Struct. contains planar, hexagonal, graphite like layers of B stacked alternately with hcp layers of Mn (like AlB_2). Obt. from the elements by arc melting. Metallic conductor. Grey-violet cryst. Mp 1988°.

Antiferromagnetic; weakly ferromagnetic at T_c 157K. At 800° → MnB_4 + Mn_3B_4.

Manganese boride* (MnB_4), *11CI [12271-96-4]

B_4Mn M 98.1

Monoclinic, struct. contains a boron framework of 4-membered rings. Obt. by arc melting Mn and crystalline B. Can also be prepared from MnB_2 at 750°: $4MnB_2$ → MnB_4 + Mn_3B_4. Cryst. Mp ~2160°.

Kiessling, R., *Acta Chem. Scand.*, 1950, **4**, 146 (*cryst struct*)
Aronsson, B., *Acta Chem. Scand.*, 1960, **14**, 1414 (*synth, MnB_2*)
Lundquist, N., *Ark. Fys.*, 1962, **20**, 463 (*MnB, magnetism*)
Lundquist, N., *Philos. Mag.*, 1962, **7**, 1187 (*electronic struct, MnB*)
Márkovskii, L.Ya. *et al., J. Appl. Chem. USSR (Engl. Transl.)*, 1965, **38**, 1643 (*synth, Mn_3B*)
Hohnke, H. *et al., Acta Crystallogr.*, 1966, **20**, 572 (*cryst struct, MnB*)
Bezrukh, E.T. *et al., J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 873 (*synth*)
Andersson, S. *et al., Acta Chem. Scand.*, 1970, **24**, 1791 (*synth, cryst struct MnB_4*)
Kasaya, M. *et al., J. Phys. Soc. Jpn.*, 1970, **29**, 336; 1971, **30**, 286 (*magnetism*)
Ward, R., *MTP Int. Rev. Sci., Inorg. Chem., Ser. One*, 1972, **5**, 93 (*cryst struct, Mn_4B_4*)
Brown, P.J. *et al., The Crystal Structure of Solids*, London, 1973, 148 (*cryst struct, Mn_3B*)
Matkovich, V.I., *Pure Appl. Chem.*, 1974, **39**, 525 (*cryst struct*)
Nemoshkalenko, V.V. *et al., J. Phys. Chem. Solids*, 1975, **36**, 37 (*pe, Mn_3B, MnB_2*)
Spear, K.E., *J. Less-Common Met.*, 1976, **19**, 195 (*cryst struct, MnB_2*)
Lundström, T. *et al., Boron Refract. Borides*, (Ed. Matkovich, V.I.) Berlin, 1977 (*cryst struct, MnB_2*)
Pyaseukii, I.I. *et al., CA*, 1978, **89**, 9837 (*props*)
Cely, A. *et al., J. Less-Common Met.*, 1978, **61**, 193 (*prop*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 5 (*rev, bibl*)
Ishii, T. *et al., Solid State Commun.*, 1984, **51**, 203 (*magnetism*)

[BMo] IC-000899

Molybdenum borides

[12626-91-4]

Molybdenum boride* (Mo_2B), *9CI, 8CI [12006-99-4]

BMo_2 M 202.6

Tetragonal $CuAl_2$-type struct. Synth. from BBr_3 + $MoCl_5$. Refractory. Important uses as a braze and in cutting tools. Oxidises in air on heating. Insol. H_2O. Mp 2280°, Mp 2000° dec.

Molybdenum boride* (*MoB*), *9CI, 8CI [12006-98-3]

BMo M 106.7

Dimorphic, with α- tetragonal form and β- rhombic (CrB or VB struct. type) form. Synth. from BN + Mo (CrB or VB struct. type) form. Synth. from BN + Mo at 1400-1600° or $MoCl_5$ + BBr_3. Refractory, used as braze and in cutting tools. Sol. H_2SO_4 (1:2) + HNO_3 at 150°, insol. H_2O. Mp 2550-2600° (β-form), Mp 2180°. When finely divided, begins to oxidise in air at *ca.* 650°.

Molybdenum boride* (MoB_2), *9CI, 8CI [12007-27-1]

Molybdenum diboride

B_2Mo M 117.5

Composition actually $MoB_{1.8}$-$MoB_{2.0}$. Has the hexagonal AlB_2-type struct. Synth. from Mo_2B_5 at >1600° or elements. Refractory, used in braze and in cutting tools. Oxidises in air on heating. Mp 2350°, Mp 2300° (2100°) dec.

Molybdenum boride* (Mo_2B_5), *9CI, 8CI [12007-97-5]

B_5Mo_2 M 245.9

Rhombic. Synth. from Mo_2O_3 + B_2O_3 + Mg at 1200°, MoO_2 + B_4C + C, or elements at 1200-1500°. Mp 2315° (2100°). At >1600° → MoB_2. Stable to HCl (1:1), H_2SO_4 (1:1), 5-20% aq. NaOH. Attacked by fused NaOH. Dec. by 30% H_2O_2 and acids containing H_2O_2.

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Molybdenum boride* (MoB_4), *9CI, 8CI [12265-21-3]

B_4Mo M 139.1

Tetragonal, isomorphous and isodimensional with WB_4. UB_4-type struct.

Molybdenum boride* (MoB_{12}), *9CI, 8CI [12305-71-4]

Molybdenum dodecaboride

$B_{12}Mo$ M 225.6

Hexagonal. Observed in Mo—W—B ternary system.

Kiessling, R., *Acta Chem. Scand., Ser. A*, 1947, **1**, 893 (*struct, MoB, Mo_2B, Mo_2B_5*)
Cheriom, A. *et al., Compt. Rend. Hebd. Seances Acad. Sci.*, 1961, **252**, 742 (*synth*)
Rudy, E. *et al., Z. Metallk.*, 1963, **54**, 345 (*synth, phase diagram, structs*)
Funke, V.F. *et al., Zh. Prikl. Khim. (Leningrad)*, 1963, **36**, 2379; *J. Appl. Chem. USSR (Engl. Transl.)*, 1963, **36**, 2308 (*synth*)
Probst, P. *et al., J. Less-Common Met.*, 1967, **13**, 241 (*synth*)
Kerrand, G., *Chim. Ind., Genie Chim.*, 1968, **99**, 900; *CA*, **69**, 21592 (*synth, props*)
Lundström, T., *Ark. Kemi.*, 1969, **31**, 227 (*struct, MoB_2*)
Meerson, G.A. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 2079; *Inorg. Materials (Engl. Transl.)*, 1969, **5**, 1767 (*purif*)
Markovskii, L.Ya. *et al., Poroshk. Metall. (Kiev)*, 1969, **9**, 13; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, **9**, 350.
Khartsonov, V.I. *et al., Poroshk. Metall. (Kiev)*, 1969, **9**, 60; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, **9**, 567 (*synth*)
Storey, R.N. *et al., J. Crystal Growth*, 1970, **6**, 261.
Kuzma, L.N. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 769; *Inorg. Materials (Engl. Transl.)*, 1972, **8**, 669 (*props*)
Cruel, B.B. *et al., J. Chem. Phys.*, 1972, **56**, 1549 (*nqr, cryst struct*)
Ismail, G. *et al., Monatsh. Chem.*, 1973, **104**, 266 (*synth, MoB_2*)
Mayell, G. *et al., Surf. Sci.*, 1973, **35**, 109 (*pe*)
Armas, B., *Rev. Int. Hautes Temp. Refract.*, 1975, **12**, 255; 1976, **13**, 49 (*synth*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Matsumoto, O. *et al., High Temp. Sci.*, 1978, **10**, 175 (*synth, pe, struct*)
Aleshin, V.G. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1979, **15**, 672; *Inorg. Materials (Engl. Transl.)*, 1979, **15**, 525 (*pe*)

BN

Boron nitride (BN) IC-000900

[10043-11-5]

BN

M 24.8

Primarily found in a hexagonal form (α-BN). Zinc blende-type (β-BN) and wurtzite-type (γ-BN) forms also exist. Commercially available.

α-form

Prepd. by igniting B compds. with N compds. Used as a ceramic, e.g. for crucibles. Soft white powder. Struct. resembles that of graphite except that the rings in one layer are stacked directly on top of the rings in adjacent layers. Insol. H_2O. Subl. 2330° (under nitrogen).

β-form

Borazon

Formed from α-BN at 85000 atm. and 1800°. An abrasive. Colourless when pure. V. hard. Structure is related to that of cubic diamond.

γ-form

Formed by static compression of α-BN at 11.5-12 × 10^4 atm. and ≤600° or by shock compression up to 5.5 × 10^5 atm. Structure is related to that of hexagonal diamond.

Pease, R.H., *Acta Crystallogr.*, 1952, **5**, 356 (*cryst struct*)
Wentorf, R.H., *J. Chem. Phys.*, 1957, **26**, 956; 1961, **34**, 809 (*synth, sphalerite-form*)
Silver, A.H. *et al., J. Chem. Phys.*, 1960, **32**, 288 (*B-11 nmr*)
O'Connor, T.E., *J. Am. Chem. Soc.*, 1962, **84**, 1753 (*synth*)
Soma, T. *et al., Mater. Res. Bull.*, 1974, **9**, 755 (*synth, wurtzite-form*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 805 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **15**, 873 (*rev*)
Merck Index, 11th Ed., 1989, No. 1348.
Paine, R.T. *et al., Chem. Rev.*, 1990, **90**, 73 (*rev*)

BN_9

Boron azide, 9CI IC-000901

[21884-15-1]

$B(N_3)_3$

M 136.8

Synth. from BH_3 + $3HN_3$.

Py complex (1:1): Colourless liq. Bp 130° in high vacuum.

Wiberg, E. *et al., Z. Naturforsch., B*, 1954, **9**, 497 (*synth*)
Paetzold, P.I., *Z. Anorg. Allg. Chem.*, 1963, **326**, 58 (*synth*)

$BNaO_2$

Sodium metaborate IC-000902

Boric acid (HBO_2), sodium salt, 8CI. Sodium polydioxoborate(III). Polydioxoboric(III) acid, sodium salt

[7775-19-1]

$NaBO_2$

M 65.8

The Na_2O-B_2O_3 system forms an extensive series of glasses. Prepd. from $NaBH_4$ either by hydrol. or by reaction with air at 300-450°. Alternatively, it can be formed by heating equimolar quantities of Na_2CO_3 and $Na_2B_4O_7$ or

by reaction of H_3BO_3 with NaOH or Na_2CO_3. Commercially available as hydrate. Fireproofing agent. V. sol. H_2O V. hygroscopic colourless hexagonal cryst. V. sol. H_2O (26 g per 100 cm^3 at 20°, 36 g per 100 cm^3 at 35°); insol. EtOH, Et_2O. Mp 967°. Bp 1434°. ΔH_f° −976 kJ mol^{-1}; ΔG_f° −919 kJ mol^{-1}; S° 73.55 J K^{-1} mol^{-1}

α-form: see *Triborate(3−), IC-001066*

Glunk, J.C. *et al., J. Phys. Chem.*, 1932, **36**, 586 (*raman*)
Unak, T.P. *et al., J. Phys. Chem.*, 1959, **63**, 1533 (*B-11 nmr*)
Goubeau, J. *et al., Z. Phys. Chem. (Frankfurt am Main)*, 1959, **20**, 15 (*ir*)
Hart, P.B. *et al., J. Inorg. Nucl. Chem.*, 1962, **24**, 1047 (*ir*)
Marezio, M. *et al., Acta Crystallogr.*, 1963, **16**, 594 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1966, **3**, 1263 (*rev, bibl*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 248 (*thermochem data*)
Bair, R. *et al., Z. Naturforsch., A*, 1986, **41**, 737 (*B-10 nmr, B-11 nmr*)

$BNaO_3$ IC-000903

Sodium perborate ($NaBO_3$)

[7632-04-4]

$NaBO_3$

M 81.7

Anhydrous form. Prepd. by heating the tetrahydrate. Used as an oxygen source. Hygroscopic, white amorph. powder. Evolves O_2 when dissolved in H_2O.
⚠ Can be detonated by light friction.

Monohydrate. [10332-33-9]
BH_2NaO_3 M 99.8
Prepn. by heating the tetrahydrate to 60°. Bleaching agent. Strong oxidising agent. White amorph. powder. Sol. H_2O (with liberation of H_2O_2). Mp 88°. Correctly formulated as $Na_2[B_2O_3(O_2)(OH)_2]$.
Sol. 1320880

Trihydrate. [28902-63-8]
BH_7NaO_6 M 135.8
Cryst. from aq. solns. of the pure tetrahydrate. White cryst. Mp 82°. Correctly formulated as $Na_2[B_2(O_2)_2(OH)_4].4H_2O$.

Tetrahydrate: see *Sodium perborate tetrahydrate, IC-000905*

[10486-00-7; 12022-44-6]

Van Gelder, G.W. *Rec. Trav. Chim. Pays-Bas U. R. Neth. Chem. Soc.*, 1956, **75**, 137 (*synth, tetrahydrate*)
Cousins, T.M. *et al., J. Chem. Soc.*, 1959, 259 (*pmr, hydrates*)
Unak, T.P. *et al., J. Phys. Chem.*, 1959, **63**, 1533 (*B-11 nmr*)
Ekeström, A., *Acta Chem. Scand.*, 1961, **15**, 934 (*cryst struct tetrahydrate*)
Griffith, W.P. *et al., Chem. Ind. (London)*, 1984, 183 (*cryst struct tetrahydrate*)
McKillop, A. *et al., Tetrahedron*, 1987, **43**, 1753 (*use*)
Merck Index, 11th Ed., 1989, No. 8504
Flanagan, J. *et al., Spectrochim. Acta, Part A*, 1989, **45**, 951 (*synth, ir, nmr*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand Reinhold, 1989, 795

[BNb] IC-000904

Niobium borides

[12653-77-9]

***Niobium boride* (Nb_3B_2)** [12045-58-5]
B_2Nb_3 M 308.3
Tetragonal. Mp *ca.* 2000°

Niobium boride* (*NbB*), *9CI, 8CI [12045-19-1]
Niobium monoboride
BNb M 103.7
Orthorhombic CrB-type struct. Synth. from Nb_2O_5 + B_2O_3 + Mg at 1200°. Employed in refractory electrodes. Mp *ca.* 2200°.

Niobium boride* (Nb_3B_4), *9CI, 8CI [12045-89-5]
B_4Nb_3 M 321.9
Has the orthorhombic Ta_3B_4 (Mn_3B_4)-type struct. Synth. from Nb + BN at 1400-1700°. Mp *ca.* 2700°.

***Niobium boride* (NbB_2)** [12007-29-3]
Niobium diboride
B_2Nb M 114.5
Has the hexagonal AlB_2-type struct. Synth. from Nb_2O_5 + B or $NbBr_5$ + BBr_3. Mp *ca.* 3000°. Dec. by 5-20% aq. NaOH at 80°. Not attacked by HCl (1:1), HNO_3 (1:1). Dec. by H_2O_2 or acid solns. cont. H_2O_2. When finely divided, oxidation begins at *ca.* 650°.

Rudy, E. *et al., Z. Metallk.*, 1963, **54**, 345 (*synth, phase diagram, structs*)
Peshev, P. *et al., J. Less-Common Met.*, 1968, **15**, 259 (*synth, anal*)
Markovskii, L.Ya. *et al., Poroshk. Metall. (Kiev)*, 1969, **9**, 13; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, 350 (*synth*)
Kovenskaya, B.A. *et al., Poroshk. Metall. (Kiev)*, 1970, **10**, 79; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1970, 415 (*phys. props*)
Kugai, L.N. *et al., Poroshk. Metall. (Kiev)*, 1971, **11**, 51; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 212 (*props*)
Mavel, G. *et al., Surf. Sci.*, 1973, **35**, 109 (*pe*)
Samsonov, G.V. *et al., Rev. Int. Hautes Temp. Refract.*, 1974, **11**, 269 (*rev*)
Armas, B. *et al., Rev. Int. Hautes Temp. Refract.*, 1975, **12**, 255; 1976, **13**, 49 (*synth*)
Armas, B. *et al., J. Electrochem. Soc.*, 1976, **123**, 308 (*synth*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
McKee, D.W., *Carbon*, 1986, **24**, 331 (*props*)

[BNd] IC-000905

Neodymium borides

NdB_{11} appears not to have been reported; existence of NdB_{66} in doubt.

Neodymium boride* (NdB_4), *9CI, 8CI [12007-77-1]
Neodymium tetraboride
B_4Nd M 187.4
Tetragonal UB_4-type struct. Golden cryst. At 1850° *in vacuo* → NdB_6 + Nd. Antiferromagnetic.

Neodymium boride* (NdB_6), *9CI, 8CI [12008-23-0]
Neodymium hexaboride
B_6Nd M 209.1
Has the cubic CaB_6-type struct. Synth. from Nd_2O_3 + B at 1500-1800°. Blue-violet solid. Mp 2610° (2540°). Fairly unreactive to dil. HCl or H_2SO_4. Dissolves easily in aqua regia. Stable to 650-700°. Ignites at 710°. Oxidises at > 730° to $Nd(BO_2)_3$.

[37322-41-1]

Niemyski, T. *et al., J. Less-Common Met.*, 1968, **15**, 97 (*purifn*)
Mordovin, G.A. *et al., Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Kosolapova, T.Ya. *et al., Poroshk. Metall. (Kiev)*, 1970, **10**, 1; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1970, **10**, 353
Adadurov, G.A. *et al., Zh. Neorg. Khim.*, 1970, **15**, 2887; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1503 (*synth*)
Tumareeva, E.Ya. *et al., Zh. Prikl. Khim. (Leningrad)*, 1971, **44**, 1309; *J. Appl. Chem. USSR (Engl. Transl.)*, 1971, **44**, 1414 (*props*)
Etourneau, J. *et al., Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1688 (*synth*)
Buschow, K.H.J. *et al., J. Chem. Phys.*, 1972, **57**, 3910 (*magnetism*)
Fisk, Z. *et al., Mater. Res. Bull.*, 1972, **7**, 285 (*cryst struct*)
Chazalviel, J.N. *et al., Phys. Rev. Lett.*, 1976, **37**, 919 (*pe*)
Ishii, M. *et al., Solid State Commun.*, 1976, **20**, 437 (*raman*)

Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Cannon, J.F. *et al., J. Less-Common Met.*, 1977, **56**, 83 (*synth*)
Kuz'ma, Yu.B. *et al., J. Less-Common Met.*, 1983, **90**, 217.

IC-000906

[BNi]

Nickel borides

[12619-90-8]

Nickel boride* (Ni_3B), *9CI, 8CI [12007-02-2]
BNi_3 M 186.8
Has the orthorhombic Fe_3C (cementite) struct. Mp 1165°. Resistant to boiling H_2O. Reactive to 25% $HClO_4$ aq.

Nickel boride* (Ni_2B), *9CI, 8CI [12007-01-1]
BNi_2 M 128.1
Has the tetragonal $CuAl_2$-type struct. Synth. from $Ni(OAc)_2$ + $NaBH_4$ → black ppt. stored under MeOH. Hydrogenation catalyst. Mp 1230°.

Nickel boride* (Ni_4B_3), *9CI, 8CI [12045-67-9]
B_3Ni_4 M 267.1
Dimorphic. The orthorhombic Ta_3B_4 form has 3 types of interconnected Ni trigonal prisms with B atoms at centres. The monoclinic form is built up of close-packed, sl. corrugated Ni atom layers with B atom chains in the metal atom lattice. Mp 1025° (orthorhombic) 1902° 1031° (monoclinic). Resistant to boiling H_2O. Completely reactive to 25% $HClO_4$ aq.

Nickel boride* (*NiB*), *9CI, 8CI [12007-00-0]
Nickel monoboride
BNi M 69.5
Has the CrB (VB)-type struct. Synth. from NiS + BCl_3 + H_2 at 500-800°. Sol. cold aqua regia. Resistant to $HClO_4$. Part. sol. H_2SO_4 or H_3PO_4. Mp 1080°.

Nickel boride* (NiB_2), *9CI, 8CI [12045-56-6]
Nickel diboride
B_2Ni M 80.3
Component of the Ni-B system.

Kiseleva, I.D. *et al., Z. Metallk.*, 1963, **54**, 656 (*synth, phase diagram*)
Ruotsalainen, S. *et al., Acta Chem. Scand.*, 1967, **21**, 191 (*cryst struct*)
Selishev, K.S. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 123; *Inorg. Materials (Engl. Transl.)*, 1967, **3**, 663 (*synth, phase diagram*)
Portnoi, K.I. *et al., Poroshk. Metall. (Kiev)*, 1967, **7**, 15; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1967, **7**, 99 (*phase diagram*)
Timofeeva, N.I. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 1513; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 1423 (*props*)
Casteleiro, J. *et al., J. Less-Common Met.*, 1971, **24**, 317 (*synth*)
Lind, D.R. *et al., J. Chem. Phys.*, 1972, **56**, 1549 (*aqr*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Alishin, V.G. *et al., J. Less-Common Met.*, 1979, **67**, 173 (*pe*)
Lugscheider, E. *et al., Z. Metallk.*, 1980, **71**, 239 (*struct*)
Sato, S. *et al., Metall. Trans. B*, 1982, **13**, 251 (*synth*)

IC-000907

Boron oxide (BO), 11Cl, 10Cl, 9Cl

Boron monoxide

[12503-77-0]

$[BO]_n$

M 26.8

Known as gas phase radical monomer or polymeric solid. Colourless solid. Sol. MeOH, EtOH. In EtOH reduces $Ag^{\oplus}$.

Wunk, T. *et al., J. Am. Chem. Soc.*, 1955, **77**, 6400 (*synth, polymeric form*)

$BO_2^{\ominus}$ IC-000908

Metaborate(1−), 10Cl, 9Cl

[14100-65-3]

$[BO_2]^{\ominus}$

M 42.8 (ion)
Usually found as a linear chain polyanion with B—O—B bonds, $(BO_2)_n^{n\ominus}$, but v. rarely occurs as a linear $[O{=}B{-}O]^{\ominus}$ species.

Na salt: see *Sodium metaborate, IC-000902*
K salt: see *Potassium metaborate 1½ hydrate* (or *1½ hydrate*), *IC-001085*
Ca salt: see *Calcium metaborate* (CaB_2O_4), *IC-000957*
Non-stoichiometric deriv.: *Strontium sodium phosphate borate*
$B_{0.998}Na_{0.997}O_{10}P_4Sr_{2.997}$ M 144.2
Contains linear $[O{=}B{-}O]^{\ominus}$ anion.

Marezio, M. *et al., Acta Crystallogr.*, 1963, **16**, 390 (*cryst struct*)
Marezio, M. *et al., J. Chem. Phys.*, 1966, **44**, 3348 (*cryst struct*)
Kriz, H.M. *et al., J. Chem. Phys.*, 1968, **49**, 557 (*B-11 nmr*)
Calvo, C. *et al., Acta Crystallogr., Sect. B*, 1975, **31**, 188 (*cryst struct*)
Foss-Smith, D., *Spectrochim. Acta, Part A*, 1976, **32**, 319 (*ir*)

BO_2 IC-000909

Boron oxide (BO_2), 11Cl, 10Cl, 9Cl, 8Cl

Boron dioxide

[13840-88-5]

BO_2

M 42.8
Gas phase radical.

Simmons, A. *et al., J. Chem. Phys.*, 1963, **38**, 87 (*synth, ir*)
Bauer, S.H. *et al., IEEE J. Quantum Electron.*, 1978, **14**, 237; *C.A.* **88**, 200278 (*synth*)
Jasuja, M.L., *J. Phys. Chem. Ref. Data*, 1984, **13**, 945 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *3rd Suppl.*, 1987, **3**, 7 (*rev, bibl*)

$BO_3^{3\ominus}$ IC-000910

Borate(3−), 10Cl, 9Cl

[14213-97-9]

$[BO_3]^{3\ominus}$

M 58.8 (ion)
Trigonal planar anion.

Tri-Li salt: [13774-56-6]. *α-Lithium borate* (Li_3BO_3)
BLi_3O_3 M 79.6
Colourless cryst. Possesses typical monomeric $(BO_3)^{3\ominus}$ struct.

Siewner, F., *Acta Crystallogr., Sect. B*, 1971, **27**, 904 (*cryst struct*)
Kobetz, E., *Z. Kristallogr.*, 1982, **160**, 81 (*rev*)
Zehnder, E.J. *et al., CA*, 1983, **98**, 224551 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *Suppl. Vol.* 3, 1987, **2**, 48 (*rev, bibl*)

BO_3V IC-000911

Vanadium(*III*) borate (VBO_3)

VBO_3

M 109.7
Calcite-like struct. Synth. by a complex vapour phase process from B_2O_3, V_2O_3 + V; VCl_3. Red-brown solid.

Schmidt, H., Acta Crystallogr., 1964, **17**, 1080 (*synth, cryst struct*)

BO_4P IC-000912

Boron phosphate, 11Cl, 10Cl, 9Cl

[13308-51-5]

BPO_4

M 26.8
Solid has a polymeric struct. of linked BO_4 and PO_4 tetrahedra. Commercially available. Catalyst in org. reactions (eg. dehydrates EtOH to C_2H_4 + Et_2O). Colourless solid.

▷ Irritant.

Bray, P.J. et al, J. Chem. Phys., 1961, **35**, 435 (*B-11 nmr*)
Weir, C.E. et al, J. Res. Natl. Bur. Stand., Sect. A, 1964, **68**, 465 (*ir*)
Moffat, J.B. et al, J. Catal., 1973, **31**, 274; 1974, **34**, 376 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, Boron Compds., 1975, **3**, 99 (*rev, bibl*)
Turner, G.L. et al, J. Magn. Reson., 1986, **67**, 544 (*B-11 nmr*)

$BO_{39}W_{11}^{9\ominus}$ IC-000913

Tungstoborate ($BW_{11}O_{39}^{9\ominus}$)

Eicosa-μ-oxopentadecaoxo[μ_{11}-[tetrahydroxyborato(5−)]]undecatungstate(9−), 10CI

[61512-29-6]

$[BW_{11}O_{39}]^{9\ominus}$

M 2657.1 (ion)
A Keggin-type heteropolyanion. Prepared by base degradation of $[BW_{12}O_{40}]^{5\ominus}$

[81553-05-1]

Souchay, P., Ann. Chim., 1945, **20**, 73 (*synth*)
Tourne, C. et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C., 1968, **266**, 702, 1363 (*synth*)
Fu, G. et al, Yingyong Huaxue, 1989, **6**, 16, C.A. **112**, 227867g (*crystal struct*)

$BO_{40}ReW_{11}^{4\ominus}$ IC-000914

Rhenatungstoborate ($BReW_{11}O_{40}^{4\ominus}$)

Polybarotetrarhenatungstate(4−), 11-Tungstorhenborate(4−)

$[BW_{11}ReO_{40}]^{5\ominus}$

M 2859.3 (ion)
Contains Re(VII). Heteropolyanion with a Keggin struct.
Tetrakis-tetrabutylammonium salt: [91741-66-1]
Synth. from $Na_9BW_{11}O_{39}$ and $[ReO_3Py_4]Br.2H_2O$ in buffered H_2O followed by $[Bu_4N]Br$. Yellow cryst.

Herve, F. et al, Inorg. Chem., 1988, **23**, 3292 (*synth, struct, electrochem, spectr, stab, ir, props*)

$BO_{40}W_{12}^{5\ominus}$ IC-000915

Tungstoborate ($BW_{12}O_{40}^{5\ominus}$), 8CI

Tungstate. Tetracosa-μ-oxododecaoxo[μ_{12}-12-Borotungstate. Tetracosa-μ-oxododecaoxo[μ_{12}-[tetrahydroxyborato(5−)]]dodecatungstate(5−), 10CI

[12513-03-0]

$[BW_{12}O_{40}]^{5\ominus}$

M 2856.9 (ion)
A Keggin-type heteropolyanion. Prepd. by heating $[WO_4]^{2\ominus}$ with H_3BO_3 in aq. HCl.

Penta-K salt: [11078-54-9].
Cryst. (H_2O).

Penta-H compd.: see *Tungstoboric acid* ($H_5BW_{12}O_{40}$), *IC-000879*

Tetrakis-tetrabutylammonium salt, H compd.: [83844-83-1].
Solid + H_2O ($MeCN/Et_2O$).

[12045-18-0, 112763-08-3]

Rashkin, J.A. et al, J. Phys. Chem., 1967, **71**, 1265 (*cryst struct*)
Acerete, R. et al, J. Am. Chem. Soc., 1982, **104**, 5384 (*W-183 nmr*)
Rocchiccioli-Deltcheff, C. et al, Inorg. Chem., 1983, **22**, 207 (*synth, ir, raman, electrochem*)
Piepgrass, K. et al, J. Am. Chem. Soc., 1987, **109**, 1586 (*W-183 nmr*)
Nomiya, K. et al, Polyhedron, 1987, **3**, 519 (*uv*)

BP IC-000916

Boron phosphide (BP), 9CI

[20205-91-8]

BP

M 41.7
Has the zinc-blende struct. Prepd. by direct union of B and red P at ~ 1000° in a reducing atm. Several other methods of prepn. have been reported. Commercially available. Semiconductor. Refractory maroon powder. Insol.

▷ Ignites at 200°. Emits toxic fumes in contact with H_2O and acids.

Perri, J.A. et al, Acta Crystallogr., 1958, **11**, 310 (*cryst struct*)
Williams, F.W. et al, J. Am. Chem. Soc., 1960, **82**, 1330 (*synth*)
Weilleron, J. et al, Bull. Soc. Chim. Fr., 1965, 402; 1968, 3204 (*synth*)
Kuchio, W., Z. Anorg. Allg. Chem., 1967, **349**, 151 (*synth*)
Sax, N.I. et al, Dangerous Properties of Industrial Materials, 7th Ed., Van Nostrand-Reinhold, 1989, 546

[BPd] IC-000917

Palladium borides

Palladium boride (Pd_3B), 9CI, 8CI [12429-53-7]
BPd_3 M 330.0
Has the Fe_3C (cementite)-type struct. Composition nearer to $Pd_{3.25}B$. Synth. from Pd + B at 1400-1500° and from $Pd(MeCN)_2Cl_2$ in toluene with B in K. Mp 1110° (820°).

Palladium boride (Pd_2B_3), 9CI, 8CI [11130-91-9]
B_3Pd_2 M 533.7
Composition nearer to $Pd_{1.25}B_3$. Monoclinic lattice. Corrugated layers of Pd atoms at corners of interconnected squares and triangles. B atoms at centres of hexagonal prisms. Synth. from Pd + B at 800-900°. Mp 1190° (870°).

Stenberg, E., Acta Chem. Scand., 1961, **15**, 861 (*synth, cryst struct*)
Samsonov, G.V. et al, Zh. Prikl. Khim. (Leningrad), 1971, **44**, 2369; *J. Appl. Chem. USSR (Engl. Transl.)*, 1971, **44**, 2552 (*synth*)

Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Carturan, G. et al, React. Solids, 1985, **1**, 31 (*synth*)

[BPr] IC-000918

Praseodymium borides

Thought not to form PrB_{66} phase.

Praseodymium boride (PrB_4), 9CI, 8CI [12007-78-2]
B_4Pr M 184.1
Has the tetragonal UB_4-type struct. Black cryst. Ferromagnetic (T_c 25K). Dissoc. → PrB_6 at 1950° in high vacuum.

Praseodymium boride (PrB_6), 9CI, 8CI [12008-27-4]
Praseodymium hexaboride
B_6Pr M 205.7
Has the cubic CaB_6-type struct. Synth. from the oxide + B at 1500-1800°. Blue solid. Mp 2610° dec. Fairly stable to dil. acids. Dissolves in HNO_3 or conc. H_2SO_4 with dec. When melted → PrB_4. Undergoes phase transitions at 6.9K and 4.2K.

Niemyski, T. et al, J. Less-Common Met., 1968, **15**, 97 (*purifn*)
Mordovin, O.A. et al, Zh. Neorg. Khim., 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Kosolapova, T.Ya. et al, Poroshk. Metall. (Kiev), 1970, **10**, 1; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1970, **10**, 353 (*props*)
Etourneau, J. et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C, 1972, **274**, 1688 (*synth*)
Fisk, Z. et al, Mater. Res. Bull., 1972, **7**, 285 (*synth, cryst struct*)
Ames, L.L. et al, High Temp. Sci., 1975, **7**, 44 (*ms*)
Ishii, M. et al, Solid State Commun., 1976, **20**, 437 (*raman*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Etourneau, J. et al, J. Less-Common Met., 1979, **67**, 531; 1985, **110**, 267 (*magnetism, electrical props, synth*)
McCarthy, C.M. et al, Solid State Commun., 1980, **36**, 861 (*nd. struct, phys props*)
Sugawara, H. et al, J. Phys. Soc. Jpn., 1982, **51**, 915 (*pe*)
Davis, P.R. et al, J. Mater. Sci., 1986, **21**, 825 (*synth, anal*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1990, **C11a**, 6 (*rev*)

[BPt] IC-000919

Platinum borides

Two phases, Pt_2B and Pt_4B reported.

Platinum boride (Pt_2B) [12228-36-3]
BPt_2 M 400.9
Has AlB_2 type struct. built up of close packed layers of metal atoms and B atoms arranged in trigonal prismatic geometry around each Pt atom forming three types of layers of B atoms. Synth. by electrochem. redn. of borate anion with Pt electrode.

Hassler, E. et al, J. Less-Common Met., 1979, **67**, 567 (*synth, cryst struct*)
Gonzalez, M. et al, Electrochim. Acta, 1984, **29**, 737 (*synth*)

[BRe] IC-000920

Rhenium borides

Re_3B has also been reported.

Rhenium boride (Re_3B_2), 9CI, 8CI
B_2Re_3 M 1323.0
Struct. composed of octahedra, tetrahedra and trigonal prisms of Re atoms. Synth. from elements.
Commercially available. A superconductor at 1.08K.

Rhenium boride (ReB_2), 9CI, 8CI [12355-99-6]
B_2Re M 207.8
Hexagonal cell. Struct. has alternating planar layers of Re atoms and puckered B atom layers. Synth. from elements. Mp ca. 2400° (2280°).

Aronsson, B. et al, Acta Crystallogr., 1961, **15**, 878 (*cryst struct*)
La Placa, S. et al, Acta Crystallogr., 1962, **15**, 97 (*cryst struct*)
Portnoi, K.I. et al, Poroshk. Metall. (Kiev), 1968, **8**, 41; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, 112 (*constit, phase diagram*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Chupnik, I.M., Phys. Status Solidi A, 1977, **41**, K71 (*prepn*)
Kashif, M. et al, CA, 1986, **104**, 13297 (*cryst struct*)

[BReU] IC-000921

Rhenium uranium borides

Rhenium uranium boride ($ReUB_3$) [107069-58-9]
B_3ReU M 456.6
Hexagonal. Isol. from the U—Re—B phase system.

Rhenium uranium boride ($ReUB_4$) [56994-90-9]
B_4ReU M 467.4
Isotypic with $ThMoB_4$. Synth. from B, Re and U at 1700°.

Rhenium uranium boride (ReU_2B_6) [107069-62-5]
B_6ReU_2 M 727.1
Y_2ReB_6 type. Isol. from the U—Re—B phase system.

Rogl, P. et al, Monatsh. Chem., 1975, **106**, 587 (*synth, struct*)
Val'ovka, I.P. et al, Poroshk. Metall. (Kiev), 1986, **30**, C.A. **106**, 108676w (*phase equil, struct*)

[BReY] IC-000922

Rhenium yttrium borides

Rhenium yttrium boride ($Re_{11}YB$), 10CI [62339-28-0]
$BRe_{11}Y$ M 2147.9
bcc lattice. Isol. from the B—Re—Y phase system.

Rhenium yttrium boride ($ReYB_4$) [12523-84-1]
B_4ReY M 318.3
Isostructural with $YCrB_4$. From B—Re—Y system.

Rhenium yttrium boride (ReY_2B_6), 10CI [37233-87-7]
B_6ReY_2 M 428.8
Orthorhombic, related to $YCrB_4$ struct. Synth. from alloy of same composition at 1000°. Similar Tm, Tb compds.

Rhenium yttrium boride (ReY_3B_4), 10CI [71966-71-7]
B_4ReY_3 M 496.1
Isol. from the Y—Re—B phase system.

Rhenium yttrium boride (Re_3YB_3)
B_3Re_3Y M 876.9

Rhenium yttrium boride (ReY_2B_3), 10CI [71736-66-2]
B_3ReY_2 M 418.0
Isol. from the Y—Re—B phase system.

Rhenium yttrium boride (ReY_3B_3), 10CI [61246-03-5]
B_3ReY_3 M 528.6
Orthorhombic. Isol. from the Y—Re—B system, in equilibrium with $YRe_{2-x}YB_2$, Y and Y_2ReB_6.

Mikhalenko, S.I. et al, CA, **91**, 199648j (*phase studies, prepn*)
Kuz'ma, Yu.B., Dopov. Akad. Nauk Ukr. RSR, Ser. A: Fiz. Mat. Tekh. Nauki, 1972, **34**, 160, C.A. **76**, 132357t (*ReYB4*)
Kuz'ma, Yu.B. et al, Kristallografiya, 1972, **17**, 630 (*constit, cryst struct*)
Kuz'ma, Yu.B. et al, Dopov. Akad. Nauk Ukr. RSR, Ser. A: Fiz. Mat. Tekh. Nauki, 1976, 1029, C.A. **86**, 82023 (*cryst struct*)
Mikhalenko, S.I. et al, Poroshk. Metall. (Kiev), 1977, **10**, C.A. **86**, 129121q (*synth, struct ReYB4*)
Mikhalenko, S.I. et al, Fizicheskie Svoystva Boridov, (Kuznetsova T.Ya., Ed.), Izd. Naukova Dumka, Kiev, USSR, 1978, 72, C.A. **89**, 6682 (*phases, props*)

BRe_4Zr_9 IC-000923

Rhenium zirconium boride (Re_4Zr_9B)

[51680-87-6]

Re_4Zr_9B

M 1576.6

κ phase analogous to Co_2Al_5 and Mn_3Al_{10}. Synth. from B, Re and Zr at 1200°. Alloy.

Rogl, P. *et al*, *Monatsh. Chem.*, 1973, **104**, 1497 (*synth, struct*)

[BRh] IC-000924

Rhodium borides

[11129-95-6]

A rhodium boride prep. has been employed in hydrogenation of nitriles.

Rhodium boride* (Rh_3B_2), *9CI, 8CI [11089-99-9]

B_2Rh_3 M 752.7

Struct. composed of octahedra, tetrahedra and trigonal prisms of Rh atoms. Synth. from elements.

Rhodium boride* (Rh_3B_4), *9CI, 8CI [80891-55-0]

B_4Rh_3 M 557.7

Hexagonal lattice. Struct. composed of close packed layers of Rh atoms with B atoms in octahedral holes. Synth. from elements.

[12523-58-9, 60861-45-2]

Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

Nolâng, B.I. *et al*, *J. Less-Common Met.*, 1981, **82**, 303 (*synth, cryst struct*)

Khashfi, M. *et al*, *CA*, 1986, **104**, 13297 (*cryst struct*)

Gauem, B. *et al*, *Chem. Rev.*, 1986, **86**, 763 (*use*)

[BRu] IC-000925

Ruthenium borides

The Ru-B system also contains $Ru_{11}B_8$ phase.

Ruthenium boride* (Ru_7B_3), *9CI, 8CI

B_3Ru_7 M 739.9

Formerly designated Ru_2B. Ru skeleton mainly tetrahedra, but also octahedra, and with B atoms in larger (octahedral) holes. Synth. from elements or from RuB at 930°. Superconductive at 3.38K.

Ruthenium boride* (*RuB*), *9CI, 8CI [12523-59-0]

Ruthenium monoboride

BRu M 111.8

Hexagonal WC struct. Synth. from B + Ru at 1200-1300°. Mp *ca.* 1600° (1520°). At 950° → Ru_7B_3.

Ruthenium boride* (Ru_2B_3), *9CI, 8CI [12356-00-2]

B_3Ru_2 M 234.5

Hexagonal lattice. Synth. from Ru + B at 1200-1300°. Mp 1600°

Ruthenium boride* (RuB_2), *9CI, 8CI [12360-00-8]

Ruthenium diboride

B_2Ru M 122.6

Orthorhombic. Synth. from B + Ru at 1200-1300°. Mp *ca.* 1600° dec.

Aronsson, B., *Acta Chem. Scand.*, 1959, **13**, 109; 1963, **17**, 2036 (*cryst struct*)

Obrowski, W., *Metall (Berlin)*, 1963, **17**, 108 (*phase diagram, bibl*)

Auwera-Mahieu, A.V. *et al*, *Trans. Faraday Soc.*, 1970, **66**, 809 (*ms*)

Samsonov, G.V. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1973, **46**, 1177; *J. Appl. Chem. USSR (Engl. Transl.)*, 1973, **46**, 1261 (*synth*)

Potzel, W. *et al*, *J. Solid State Chem.*, 1974, **9**, 380 (*mössbauer*)

Vandenberg, J.M. *et al*, *Mater. Res. Bull.*, 1975, **10**, 889 (*electrical props*)

Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

BS IC-000926

Boron sulfide (BS), 9CI

[12228-39-6]

BS

M 42.8

Identified in the gas phase by spectroscopy. Its existence in the solid state has not been confirmed. Identified in B_2S_3 vapour.

McDonald, J.K. *et al*, *J. Mol. Spectrosc.*, 1969, **29**, 251 (*uv*)

Gingerich, K.A., *J. Chem. Soc., Chem. Commun.*, 1970, 580 (*formn, thermodyn*)

Brom, J.M. *et al*, *J. Chem. Phys.*, 1972, **57**, 3379 (*esr*)

Jenouvrier, A. *et al*, *Can. J. Phys.*, 1981, **59**, 1851, 1862 (*uv*)

[BSc] IC-000927

Scandium borides

Scandium boride* (ScB_2), *9CI, 8CI [12007-34-0]

Scandium diboride

B_2Sc M 66.5

Has the AlB_2-type struct. Synth. from Sc_2O_3 + B when heated in high vacuum. Mp 2250°.

Scandium boride* (ScB_6), *9CI, 8CI [12785-49-8]

Scandium hexaboride

B_6Sc M 109.8

Thought to have the CaB_6-type struct. Synth. from Sc_2O_3 + B at 1800°. A tetragonal dodecaboride has also been reported.

Peshev, P., *Rev. Int. Hautes Temp. Refract.*, 1967, **4**, 289 (*synth*)

Peshev, P. *et al*, *Mater. Res. Bull.*, 1970, **5**, 319 (*synth*)

Carter, G.C. *et al*, *J. Phys. Chem. Solids*, 1971, **32**, 2415 (*Sc-45 nmr, B-11 nmr*)

Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

Aleshin, V.G. *et al*, *J. Less-Common Met.*, 1979, **67**, 173 (*pe*)

BSe IC-000928

Boron selenide (BSe)

Selenoxoborane(2), 9CI

[29750-36-5]

BSe

M 89.7

Identified spectroscopically; may be dubious. Formed from B powder + Se at 2400° in the combustion tube of a high-temp. vacuum graphite tube furance.

Puri, S.N. *et al*, *Acta Phys. Pol. A*, 1975, **47**, 533 (*mol spectrum*)

[BSi] IC-000929

Boron silicides

Silicon borides

[37299-94-8]

Boron silicide* (B_6Si), *9CI, 8CI [12008-29-6]

Silicon hexaboride

B_6Si M 92.9

Orthorhombic cell containing individual as well as interconnected icosahedra and isolated Si and B atoms. Synth. from B_2O_3 + Si or B + Si at 1600° under Ar.

Potential use in nuclear reactor control rods. Black cryst. Mp 1980° dec. (1860°). Reacts with Cl_2 at red heat. Acted on by boiling HNO_3. Unreactive to fused KNO_3. Rapidly attacked by alkali-carbonate melts.

Boron silicide* (B_4Si), *9CI, 8CI [12007-81-7]

Silicon tetraboride

B_4Si M 71.3

Isotypic with B_4C. Synth. from Si + B_2O_3, or Si + B at 2000-2500°. Potential use as blast-furnace lining and in nuclear reactor control rods. Mp 1870° dec. Unstable when heated in air → orthorhombic B_6Si.

***Boron silicide* (B_3Si)** [12007-50-0]

Silicon triboride

B_3Si M 60.5

Now thought to be identical to B_4Si.

***Boron silicide* (*BSi*)** [12589-02-5]

Silicon boride (SiB)

BSi M 38.8

[12589-02-5]

Matkovich, V., *Acta Crystallogr.*, 1960, **13**, 679 (*struct*)

Lamikhov, L.K., *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1076; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 945 (*phase diagram, synth, bibl*)

Rai-Chaudhury, P. *et al*, *J. Crystal Growth*, 1970, **7**, 361 (*synth*)

Bremser, W. *et al*, *Chem.-Ztg.*, 1972, **96**, 36 (*pe*)

Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

Lugscheider, E. *et al*, *Ber. Dtsch. Keram. Ges.*, 1979, **56**, 301 (*phase diagram*)

McKee, D.W., *Carbon*, 1986, **24**, 331 (*props*)

Vlasse, M. *et al*, *J. Solid State Chem.*, 1986, **63**, 31 (*synth, cryst struct*)

[BSm] IC-000930

Samarium borides

SmB_{12} appears not to have been reported.

Samarium boride* (SmB_4), *9CI, 8CI [12007-82-8]

Samarium tetraboride

B_4Sm M 193.6

Has the tetragonal UB_4-type struct. Bluish cryst. Antiferromagnetic at low temp. Metallic props. Dissociates *in vacuo* at 1650°.

Samarium boride* (SmB_6), *9CI, 8CI [12008-30-9]

Samarium hexaboride

B_6Sm M 215.2

Has the cubic CaB_6-type struct. Possesses an intermediate valence state ($Sm^{2\oplus}/Sm^{3\oplus}$). Synth. from Sm_2O_3 + B at 1500-1800°. V. thin bluish-black needles or platelets. Mp 2580° (2400°). Semiconductor. Dissoc. completely when heated. Stable to 650-700°, but ignites at 693°.

Samarium boride* (SmB_{66}), *9CI [37322-42-2]

$B_{66}Sm$ M 863.8

Struct. contains B_{12} icosahedron surrounded by 12 B_{12} linked icosahedra. Unit cell contains 1584 B atoms and 24 Sm atoms. Synth. from elements. Mp *ca.* 2150°. V. hard and refractory.

Timofeeva, N.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1789; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1559 (*synth*)

Mordovin, O.A. *et al*, *Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)

Niihara, K., *Bull. Chem. Soc. Jpn.*, 1971, **44**, 963 (*synth, anal, cryst struct*)

Nickerson, J.C. *et al*, *Phys. Rev. B*, 1971, **5**, 2030 (*electronic struct, rev*)

Timofeeva, E.N. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1971, **44**, 1400; *J. Appl. Chem. USSR (Engl. Transl.)*, 1971, **44**, 1414 (*props*)

Schwetz, K. *et al*, *J. Less-Common Met.*, 1972, **26**, 99 (*synth*)

Fisk, Z. *et al*, *Mater. Res. Bull.*, 1972, **7**, 285 (*cryst struct*)

Eibschütz, M. *et al*, *Phys. Rev. B*, 1972, **6**, 18 (*mössbauer*)

Ames, L.L. *et al*, *High Temp. Sci.*, 1975, **7**, 44 (*ms*)

Chazalviel, J.N. *et al*, *Phys. Rev.*, 1976, **14**, 4586 (*pe, electronic struct*)

Ishii, M. *et al*, *Solid State Commun.*, 1976, **20**, 437 (*synth, raman*)

Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

Cannon, J.F. *et al*, *J. Less-Common Met.*, 1977, **56**, 83 (*synth*)

Gurin, V.N. *et al*, *J. Less-Common Met.*, 1979, **67**, 115 (*electrophys props*)

Aono, M. *et al*, *J. Phys. Chem. Solids*, 1979, **40**, 797 (*nqr*)

Tanaka, T. *et al*, *J. Appl. Phys.*, 1980, **51**, 3877 (*synth*)

Golikova, O.A. *et al*, *J. Less-Common Met.*, 1981, **82**, 169 (*synth, electrical props*)

Mörke, I. *et al*, *Solid State Commun.*, 1981, **40**, 331 (*raman*)

Eliseev, A.A. *et al*, *Kristallografiya*, 1986, **31**, 803; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1986, **31**, 476 (*cryst struct*)

[BSr] IC-000931

Strontium borides

Strontium boride* (SrB_6), *9CI, 8CI [12046-54-7]

Strontium hexaboride

B_6Sr M 152.4

Has the cubic CaB_6-like struct. Synth. from SrO + B, $SrCO_3$ + B, or SrF_2 + B. Dark blue (black) platelets, prisms or cubes. Mp 2235°. Semiconductor. ΔH_f° −210.9 kJ mol^{-1}.

Zhuravlev, N.N. *et al*, *Kristallografiya*, 1961, **6**, 791 (*cryst struct*)

Samsonov, G.V. *et al*, *Zh. Neorg. Khim.*, 1961, **6**, 2243 (*synth, thermodyn*)

Mamedov, F.G. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 950; *Inorg. Materials (Engl. Transl.)*, 1967, **3**, 831 (*synth*)

Peshev, P., *Rev. Int. Hautes Temp. Refract.*, 1967, **4**, 289 (*synth*)

Muranaka, S. *et al*, *J. Crystal Growth*, 1974, **26**, 165 (*synth, single cryst, cryst struct*)

Ishii, M. *et al*, *Solid State Commun.*, 1976, **20**, 437 (*raman*)

Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

Sears, R.E.J., *J. Chem. Phys.*, 1982, **76**, 5651 (*B-11 nmr*)

[BTa] IC-000932

Tantalum borides

[12653-85-9]

Tantalum boride* (Ta_3B), *9CI, 8CI [12045-26-0]

BTa_3 M 372.7

Composition closer to $Ta_{2.4}B$. Has the tetragonal $CuAl_2$-type struct. Synth. from Ta_2O_5 + B at 2000°.

Tantalum boride* (Ta_2B_3), *9CI, 8CI [12228-67-0]

B_3Ta_2 M 564.4

Said to be a constituent in the Ta-Ti-B ternary system. Composition may be closer to $Ta_{1.1}B_2$.

Tantalum boride* (*TaB*), *9CI, 8CI [12007-07-7]

Tantalum monoboride

BTa M 191.7

Orthorhombic with CrB-type struct. Synth. from BN + Mo at 1500-1700°; Ta_2O_5 + B_2O_3 + Mg at 1200°, or B + Ta_2O_5 at 1200°.

Tantalum boride* (Ta_2B_4), *9CI, 8CI [12045-92-0]

B_4Ta_2 M 586.0

Orthorhombic struct. with B atoms in double chains with B-B bonding between chains. Minor product in reaction between BN and Ta at 1500-1700°. Also synth. from Ta_2O_5 + B at 1100°.

Tantalum boride* (TaB_2), *9CI, 8CI [12007-35-1]

Tantalum diboride

B_2Ta M 202.5

Has the hexagonal AlB_2-type struct. Synth. from BBr_3 + $TaBr_5$ or Ta oxide + B at 1500-1700°. Mp *ca.* 3200°. Resistant to HCl (1:1), H_2SO_4 (1:1), HNO_3 (1:1), $HClO_4$. Slowly reacts with H_2O_2 or acids containing H_2O_2; attacked by 5-20% aq. NaOH at 80° or fused NaOH. At 1250° → TaB + B. Dissolved by HF.

Rudy, E. *et al*, *Z. Metallk.*, 1963, **54**, 345 (*phase diagram, structs*)
Peshev, P. *et al*, *J. Less-Common Met.*, 1968, **15**, 259 (*synth, anal. props*)
Samsonov, A.S. *et al*, *Poroshk. Metall. (Kiev)*, 1968, **8**, 62; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1968, **48** (*structs*)
Markovskii, L.Ya. *et al*, *Poroshk. Metall. (Kiev)*, 1969, **9**, 13; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, 350 (*synth*)
Kugai, L.N. *et al*, *Poroshk. Metall. (Kiev)*, 1971, **11**, 51; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 212 (*props, anal*)
Marek, E.V. *et al*, *Poroshk. Metall. (Kiev)*, 1971, **11**, 70; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 138 (*props*)
Borisova, A.L. *et al*, *Poroshk. Metall. (Kiev)*, 1975, **14**, 51; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1975, **14**, 822 (*synth*)
Armas, B., *Rev. Int. Hautes Temp. Refract.*, 1975, **12**, 255; 1976, **13**, 49 (*synth*)
Stümke, M. *et al*, *Z. Metallk.*, 1975, **66**, 292 (*cryst struct*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Armas, B. *et al*, *J. Crystal Growth*, 1978, **44**, 609 (*synth*)
Aleshin, V.G. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1979, **15**, 672; *Inorg. Materials (Engl. Transl.)*, 1979, **15**, 525 (*pe*)
McKee, D.W., *Carbon*, 1986, **24**, 331 (*props*)

[BTb] IC-000933

Terbium borides

TbB_{66} has been reported

Terbium boride* (TbB_4), *9CI, 8CI [12688-53-8]
Terbium tetraboride
B_4Tb M 202.1
Tetragonal UB_4-type struct. Synth. from Tb_2O_3 + B_2O_3 + Mg at 1200°. Golden cryst. Mp *ca.* 2600°. Transition to orthorhombic form at *ca.* 80K. Antiferromagnetic at low temp. $\mu_{eff} = 9.64\mu_B$.

Terbium boride* (TbB_6), *9CI, 8CI [12008-31-0]
Terbium hexaboride
B_6Tb M 223.7
Has cubic CaB_6-like struct. Synth. from Tb_2O_3 + B at 1500-1800° or Tb_2O_3 + B_2O_3 + Mg at 1200°. Cathode material. Blue solid. Mp 2340° in vapour → TbB_4 + B. $\mu_{eff} = 9.43\mu_B$.

Terbium boride* (TbB_{12}), *9CI, 8CI [12589-39-8]
Terbium dodecaboride
$B_{12}Tb$ M 288.6
Has cubic UB_{12}-like struct. Synth. from oxide + B at 1500-1700° or Tb + B at 1650° and high pressure. Antiferromagnetic.

La Placa, S. *et al*, *Acta Crystallogr.*, 1963, **16**, 1182 (*synth*)
Gordienko, S.P. *et al*, *Zh. Fiz. Khim.*, 1966, **40**, 3092; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1966, **40**, 1659 (*ms*)
Mordovin, G.A. *et al*, *Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Cannon, J.F. *et al*, *J. Less-Common Met.*, 1972, **26**, 83 (*struct, synth*)
Fisk, Z. *et al*, *Mater. Res. Bull.*, 1972, **7**, 285 (*synth, cryst struct*)
Ames, L.L. *et al*, *High Temp. Sci.*, 1975, **7**, 44 (*ms*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Bressat, B. *et al*, *J. Crystal Growth*, 1979, **47**, 429 (*synth, single cryst. cryst struct*)
Chianduzzo, J.C. *et al*, *J. Less-Common Met.*, 1981, **82**, 29 (*electrical, magnetic props*)
Golikova, O.A. *et al*, *J. Less-Common Met.*, 1981, **82**, 169

Will, G. *et al*, *J. Less-Common Met.*, 1981, **82**, 349 (*nd, struct, magnetic struct, props*)
Fisk, Z. *et al*, *Solid State Commun.*, 1981, **39**, 1189 (*magnetism*)
Hieba, Z. *et al*, *J. Phys. Chem. Solids*, 1986, **47**, 851 (*cryst structs, magnetism*)

BTe IC-000934

Boron telluride (BTe)

[29750-37-6]

BTe

M 138.4

Uy, O.M. *et al*, *High Temp. Sci.*, 1970, **2**, 293 (*ms*)

[BTh] IC-000935

Thorium borides

Compds. ThB_4, ThB_6, ThB_{12} known. ThB_{66} and ThB_{76} also reported.

***Thorium boride* (ThB_4)** [12007-83-9]
Thorium tetraboride
B_4Th M 275.2
Isoatructural with UB_4; can be non-stoichiometric. Synth. from Th + B at 1400°. Black cryst. with metallic lustre. Mp >2500°. Unreactive to O_2 below 600°. Paramagnetic.

***Thorium boride* (ThB_6)** [12229-63-9]
Thorium hexaboride
B_6Th M 296.9
Has cubic CaB_6 struct. Synth. from elements at 1500°. Potential cathode in thermionic tubes. Dark violet-black metallic cryst. or dark red powder. Insol. H_2O; sol. HNO_3. Mp 2195°.

***Thorium boride* (ThB_{12})** [37342-55-5]
$B_{12}Th$ M 361.7
ZrB_{12} or UB_{12} struct. with 12-coord. Th. Obt. by high-pressure synth.

***Thorium boride* (ThB_{66})** [12344-97-7]
$B_{66}Th$ M 945.5
Isostructural with YB_{66}. Obt. at high B/Th ratio at 1900°. Cubic cryst.

Brewer, L. *et al*, *J. Am. Ceram. Soc.*, 1951, **34**, 173
Lafferty, J.M., *J. Appl. Phys.*, 1951, **22**, 299
Zalkin, A. *et al*, *Acta Crystallogr.*, 1953, **6**, 269 (*cryst struct, ThB_4*)
Blum, P. *et al*, *Acta Crystallogr.*, 1954, **7**, 81 (*cryst struct, ThB_4*)
Post, B. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 1800 (*synth*)
Aronsson, S. *et al*, *J. Am. Ceram. Soc.*, 1967, **50**, 248 (*synth, cryst struct*)
Etourneau, J. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **266**, 1452 (*synth*)
Auskern, A.B. *et al*, *J. Chem. Phys.*, 1968, **49**, 172 (*magnetism, synth, electrical props*)
Nastasin, P. *et al*, *J. Solid State Chem.*, 1971, **3**, 101
Bushow, K.H.J. *et al*, *J. Chem. Phys.*, 1972, **57**, 3910 (*magnetism*)
Schwetz, K. *et al*, *J. Less-Common Met.*, 1972, **26**, 99
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1159 (*synth ThB_4,ThB_6*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Cannon, J.F. *et al*, *Rare Earths Mod. Sci. Technol.*, 1977, **13**, 219
Anderson, S. *et al*, *Z. Kristallogr.*, 1982, **158**, 133 (*cryst struct*)
Cannon, J.F. *et al*, *J. Less-Common Met.*, 1983, **92**, 159
Gmelin Handbook Inorg. Chem., Syst. No. 44, Suppl. Vol., 1986, **C5**, 119 (*rev*)

[BTl] IC-000936

Titanium borides

[12673-91-5]

In addition to the phases described here, Ti_2B_5 has been reported.

Titanium boride* (Ti_2B), *9CI, 8CI [12305-68-9]
M 106.5
BTi_2
Synth. from TiB_2 + Zr at 1600°.

Titanium boride* (*TiB*), *9CI, 8CI [12007-08-8]
Titanium monoboride
BTi M 58.6
Has the orthorhombic FeB-type struct. Synth. from TiB_2 + Zr, or Ti. Used in lightweight armour.

Titanium boride* (TiB_2), *9CI, 8CI [12045-63-5]
Titanium diboride
B_2Ti M 69.5
Has the hexagonal AlB_2-type struct. Synth. from $TiCl_4$ + BCl_3 under H_2 at >1000°, or from Ti_2S_3 + B at 750-900°, or TiO_2 + B_2O_3 + C at 1500-1800°. Employed in refractory materials and as metal coating. Brown solid. Mp 3225° (2850°). Attacked by HCl (1:1) (→H_2), or H_2SO_4 (1:1) (→H_2, H_2S, and SO_2) and by HNO_3 (1:1). Also attacked by 5-20% aq. NaOH at 80°, or completely by NaOH-KNO_3 flux at 600-650°. V. hard, has high thermal conductivity, low resistivity, low solubility in metals at <1000°. Resistant to oxidation at 1100°. With N_2 at 1550° → TiN.

George, W.P.R. *et al*, *Phys. Status Solidi*, 1967, **21**, 203 (*synth, electrical props*)
Markovskii, L.Ya. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1824; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1752 (*synth*)
Cueilleron, J. *et al*, *J. Less-Common Met.*, 1971, **24**, 317 (*synth*)
Minamisono, T. *et al*, *J. Phys. Soc. Jpn.*, 1971, **30**, 311 (*B-12 nmr*)
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Mavel, G. *et al*, *Surf. Sci.*, 1973, **35**, 109 (*pe*)
Armas, B. *et al*, *J. Electrochem. Soc.*, 1976, **123**, 308 (*synth*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Logan, K.V. *et al*, *Ceram. Eng. Soc. Proc.*, 1984, **5**, 712 (*manuf*)
Kim, J.J. *et al*, *Ceram. Eng. Sci. Proc.*, 1985, **6**, 1313 (*synth, rev, props, uses*)
Abdel-Hamid, A.A. *et al*, *J. Crystal Growth*, 1985, **71**, 744 (*synth, morphology*)
McKee, D.W., *Carbon*, 1986, **24**, 331 (*props*)
Thevenot, F., *Silic. Ind.*, 1986, **51**, 17 (*uses, rev*)

[BTm] IC-000937

Thulium borides

TmB_{66} has been reported.

Thulium boride* (TmB_4), *9CI, 8CI [12310-47-3]
Thulium tetraboride
B_4Tm M 212.1
Has the tetragonal UB_4-type struct. Golden cryst. Exhibits two magnetic transitions. $\mu_{eff} = 7.68\mu_B$.

Thulium boride* (TmB_6), *9CI, 8CI [12046-55-8]
Thulium hexaboride
B_6Tm M 233.8
Has the cubic CaB_6-like struct. In vap., dissociates to TmB_{12} + B.

Thulium boride* (TmB_{12}), *9CI, 8CI [12589-40-1]
Thulium dodecaboride
$B_{12}Tm$ M 298.6
Has UB_{12}-type struct. Synth. from Tm_2O_3 + B at 1450-1600°; or Tm_2O_3 + B_2O_3 + Mg at 1200°. Resistant to HCl, H_2SO_4 and dec. only by oxidising acids (*aqua regia*, cold HNO_3).

Fisk, Z. *et al*, *Mater. Res. Bull.*, 1972, **7**, 285 (*synth, cryst struct*)
Ames, L.L. *et al*, *High Temp. Sci.*, 1975, **7**, 44 (*ms*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Golikova, O.A. *et al*, *J. Less-Common Met.*, 1981, **82**, 169
Fisk, Z. *et al*, *Solid State Commun.*, 1981, **39**, 1189 (*magnetism*)
Iga, F. *et al*, *Solid State Commun.*, 1984, **50**, 903 (*synth, pe*)

[BU] IC-000938

Uranium borides

[100502-82-7]

***Uranium boride* (UB_2)** [12007-36-2]
B_2U M 259.6
Isostructural with AlB_2. Catalyst for epoxidation of olefins. Nuclear reactor fuel. Metallic solid. Mp 2365°.

***Uranium boride* (UB_4)** [12007-84-0]
Uranium tetraboride
B_4U M 281.2
Isostructural with CeB_4. Tetragonal cell. Struct. is a hybrid of MB_2/MB_6 struct. types. Each U has 5 U atoms in its own planar layer. Between these layers are 3 U atoms above and 3 U atoms below. Boron present as B_6 octahedra. Synth. from elements or UF_4 + B or UF_4 + U_3O_8 + B at 1500°; UO_3 + B at 1300° - 1500°. Nuclear reactor fuel. Metallic solid. Sol. H_2O_2/HNO_3. Attacked slowly by hot conc. H_2SO_4, not by HCl, HF.

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Blum, P. *et al*, *Acta Crystallogr.*, 1954, **7**, 81 (*struct*)
Hewlett, B.W., *J. Inst. Met.*, 1959, **88**, 91 (*synth, UB_4*)
Matkovich, V.I. *et al*, *Acta Crystallogr.*, 1965, **19**, 1056 (*cryst struct*)
Holleck, H., *J. Nucl. Mater.*, 1967, **21**, 16 (*cryst struct*)
Jeffs, J.H.E. *et al*, *J. Mater. Sci.*, 1968, **3**, 635 (*props*)
Gingerich, K.A., *J. Chem. Phys.*, 1970, **53**, 346 (*ms*)
Chechernikov, V.I. *et al*, *Fiz. Tverd. Tela (Leningrad)*, 1974, **16**, 1056; *Soviet Physics Solid State*, 1974, **16**, 681 (*magnetism*)
U.S. Pat., 4 046 784, (1975); *CA*, **88**, 120966 (*use*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1243 (*synth*)
Komac, M., *Poroshk. Metall. (Kiev)*, 1976, **15**, 97; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1976, **15**, 811 (*synth*)
Korber, V.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1977, **13**, 1660 (*stability, UB_2*)
U.S. Pat., 4 038 291, (1977); *CA*, **87**, 167859 (*use*)
U.S. Pat., 4 038 292, (1977); *CA*, **87**, 167860 (*use*)
Zhurakovskii, E.A. *et al*, *Metallofizika*, 1978, **73**, 31 (*electronic struct, UB_{12}*)
U.S. Pat., 4 203 910, (1980); *CA*, **93**, 239194 (*use*)
Mezovsky, A., *J. Crystal Growth*, 1984, **70**, 519 (*electronic prop., magnetism, cryst struct*)
Larroque, J. *et al*, *J. Less-Common Met.*, 1986, **121**, 467 (*synth, UB_2*)

[BV]

IC-000939

Vanadium borides

[12653-68-2]

Vanadium boride ***(V_2B_3), 9CI, 8CI*** [12421-53-5]
B_3V_2 M 174.4
Tetragonal lattice with U_3Si_2-type struct. Synth. from TiB_2 + V at 1300°. Mp 2060°.

Vanadium boride ***(VB), 9CI, 8CI*** [12045-27-1]
Vanadium monoboride
BV M 61.7
Has the orthorhombic CrB-type struct. Synth. from V + B in inert atm. or V_2O_3 + B_2O_3 + Mg at 1100°
Paramagnetic.

Vanadium boride ***(VB_2), 9CI, 8CI*** [12271-98-6]
B_2V M 196.0
Orthorhombic lattice, with hexagonal B atom chains and V atoms in trigonal prisms and rectangular pyramids. Ta_3B_4 struct.-type.

Vanadium boride ***(V_3B_4), 9CI, 8CI*** [12313-74-5]
B_4V_3 M 134.3
Orthorhombic lattice. Struct. based on double hexagonal B atom chains and trigonal prisms and rectangular pyramids of V atoms. Synth. from elements. Mp 2300°.

Vanadium boride ***(VB_{12}), 9CI, 8CI*** [12007-37-5]
Vanadium dodecaboride
$B_{12}V$ M 72.5
Has the hexagonal AlB_2-type struct. Synth. from (i) V_2O_5 + B_2O_3 + Mg at 1150° or (ii) V_2O_5 + B at > 1000°, or (iii) VS_2 + B at ≥ 1000°, or (iv) VCl_4 + BCl_3 under H_2. Mp 2450°. Stable to 5-20% aq. NaOH at 80°. Attacked by HCl (1:1), H_2SO_4 (1:1) (→ H_2, H_2S and SO_2), or HNO_3 (1:1).

Nowotny, H. *et al., Z. Metallk.*, 1949, **40**, 258 (*synth, phase diagram, struct*)
Rudy, E. *et al., Z. Metallk.*, 1963, **54**, 345 (*synth, phase diagram, cryst struct*)
Peshev, P. *et al., J. Less-Common Met.*, 1984, **15**, 239 (*synth, anal*)
Spear, K.E. *et al., High Temp. Sci.*, 1984, **1**, 50 (*synth, struct*)
Matkovich, V.I. *et al., Powder Metall. Met. Ceram. (Engl. Transl.)*, 1986, **25**, 158
Castanier, J. *et al., J. Less-Common Met.*, 1987, **24**, 377 (*synth*)
Kuz'ma, Yu.B. *et al., Powder Metall. Met. Ceram. (Engl. Transl.)*, 1987, **26**, 212 (*cryst struct*)
Mavel, G. *et al., Surf. Sci.*, 1973, **35**, 109 (*pe*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)

Dimorphic with hexagonal lattice or trigonal Mo_2B_5-type struct. Synth. from WO_3 + B_2O_3 + Mg at 1200°, or WO_2 + B *in vacuo* at >1300°, or WCl_6 + BBr_3. An abrasive. Mp *ca.* 2370°. Relatively stable to 5-20% aq. NaOH at 80°. Dec. accelerated by added H_2O_2.

Rudy, E. *et al., Z. Metallk.*, 1963, **54**, 345 (*synth, phase diagram, struct*)
Peshev, P. *et al., J. Less-Common Met.*, 1967, **13**, 241 (*synth*)
Portnoi, K.I. *et al., Poroshk. Metall. (Kiev)*, 1967, **7**, 75; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1967, **7**, 398 (*phase diagram, synth*)
Markovskii, L.Ya. *et al., Poroshk. Metall. (Kiev)*, 1969, **9**, 13; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1969, **9**, 350 (*synth*)
Kuz'ma, Yu.B. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 769; *Inorg. Materials (Engl. Transl.)*, 1972, **8**, 669 (*prepn*)
Creel, R.B. *et al., J. Chem. Phys.*, 1972, **56**, 1549 (*mgn*)
Kaputsev, A.I. *et al., Poroshk. Metall. (Kiev)*, 1973, **12**, 1; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1973, **12**, 777 (*manuf*)
Mavel, G. *et al., Surf. Sci.*, 1973, **35**, 109 (*pe*)
Voitovich, R.F. *et al., Poroshk. Metall. (Kiev)*, 1974, **13**, 86; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1974, **13**, 239 (*prepn*)
Armas, B. *et al., Rev. Int. Hautes Temp. Refract.*, 1975, **12**, 259; 1976, **13**, 49 (*synth*)
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[BY]

IC-000941

Yttrium borides

Yttrium boride ***(YB_2)*** [12429-58-2]
Yttrium diboride
B_2Y M 110.5
12-Coordinate hexagonal prismatic Y. Isostructural with AlB_2. Synth. from Y + B at 1000-1300° *in vacuo*. Grey cryst. Mp 2100°, Mp 1947°. Of low chemical stability. Dec. by aq. HCl.

Yttrium boride ***(YB_4)*** [12045-95-3]
Yttrium tetraboride
B_4Y M 132.1
Isostructural with UB_4. Synth. from Y_2O_3 + B at 1900° *in vacuo*. Gold metallic cryst. Insol. v. dil. HCl, but dec. by conc. HCl. Mp 2610° (2800°). Oxidises in air >760°.

Yttrium boride ***(YB_6)*** [12008-32-1]
Yttrium hexaboride
B_6Y M 153.7
Isostructural with CaB_6 composed of Y^{+9} cations and B_6 octahedra. Synth. from Y_2O_3 + B. Blue solid. Insol. v. dil. HCl. Dissolves in hot HNO_3. Mp 2600° (2300°) dec. Metallic conductor. Dec. on heating *in vacuo* above ~1500° to YB_4 + B. Chemically v. inert. Type II superconductor below 7.1K.

Yttrium boride ***(YB_{12}), 9CI, 8CI*** [12046-90-1]
Yttrium dodecaboride
$B_{12}Y$ M 218.6
Has the UB_{12}-type struct. Synth. from Y_2O_3 + B at 1500-1700°. Mp 2200° dec. Resistant to HCl or H_2SO_4, dec. by oxidising acids (cold HNO_3 or aqua regia).

Yttrium boride ***(YB_{66})*** [12280-05-6]
$B_{66}Y$ M 802.4
Complicated struct.; each unit cell has 24Y, 1548B, mainly in 13-icosahedral units. Y—B 269.1-276.8 pm. Synth. from YB_4 + B. Monochromator for soft x-ray synchotron radn. V. hard white solid (pink cast). Mp 2100°. Similar compds. formed by Nd—Lu. Stable, attacked by conc. HNO_3.

[62382-22-5]

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Johnson, R.W. *et al., J. Chem. Phys.*, 1963, **38**, 425 (*synth, YB_6, electrical props, magnetism*)

Gilles, R.F. *et al., Z. Kristallogr.*, 1965, **122**, 423 (*synth, cryst struct, YB_6*)
Rudakova, V.P. *et al., Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1966, 713 (*synth, YB_4*)
Dvorkovskii, M.V. *et al., Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1967, 93 (*synth, YB_6*)
Kuzhevskii, S.M. *et al., Acta Crystallogr., Sect. B*, 1969, **25**, 237 (*cryst struct, YB_{66}*)
Markovskii, L.Ya. *et al., Zh. Prikl. Khim. (Leningrad)*, 1969, **42**, 2690; *J. Appl. Chem. USSR (Engl. Transl.)*, 1969, **42**, 2549 (*synth, anal, pe, prepn*)
Matkovich, R.M. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 1194; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 1035 (*synth, cryst struct, prepn*)
Oliver, D.W. *et al., J. Crystal Growth*, 1971, **11**, 185 (*synth, YB_{66}*)
Carter, G.C. *et al., J. Phys. Chem. Solids*, 1971, **32**, 2415 (*B-11 nmr, T-69 nmr*)
Fisk, Z. *et al., Mater. Res. Bull.*, 1974, **9**, 633 (*struct, YB_6*)
Brandt, B. *et al., J. Crystal Growth*, 1979, **47**, 429 (*synth, single cryst, cryst struct*)
Sobczak, R.J. *et al., J. Less-Common Met.*, 1979, **67**, 167 (*synth, YB_6*)
Castro, A. *et al., Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1980, **291**, 145 (*cryst struct, YB_4*)
Tanaka, T. *et al., J. Less-Common Met.*, 1984, **102**, 281 (*synth, YB_6*)
Kumi, S. *et al., Solid State Commun.*, 1984, **52**, 659 (*conductivity, YB_6*)
Elemenko, L. *J. Less-Common Met.*, 1985, **110**, 267 (*rev, YB_6*)
Tanaka, T. *et al., J. Less-Common Met.*, 1986, **117**, 293 (*synth, prepn, YB_{66}*)
Gel'kina, O.A. *et al., J. Non-Cryst. Solids*, 1986, **87**, 64 (*synth, YB_{66}*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1990, **C11A**, 2, 6, 23, 58 (*rev*)

[BYb]

IC-000942

Ytterbium borides

Ytterbium boride ***(YbB_4), 9CI, 8CI*** [12007-85-1]
Ytterbium tetraboride
B_4Yb M 216.2
Not obt. pure. Tetragonal UB_4-like struct. Synth. from Yb_2O_3 + B + C at 1500-1800°.

Ytterbium boride ***(YbB_6), 9CI, 8CI*** [12008-33-2]
Ytterbium hexaboride
B_6Yb M 237.9
Has the cubic CaB_6-like struct. with Yb(*II*) oxidation state. Synth. from Yb_2O_3 + B at 1500-1800° or Yb_2O_3 + B_2O_3 + Mg at 1200°. Blue solid. Mp 2370°. Stable to hot aq. HCl (1:2); sol. HNO_3 (1:10) at r.t. Dissolves in H_2O at 300° under pressure. Oxid. in air at *ca.* 750°.

Ytterbium boride ***(YbB_{12}), 9CI, 8CI*** [12008-81-0]
Ytterbium dodecaboride
$B_{12}Yb$ M 302.7
Has the cubic UB_{12}-type struct. Synth. from Yb_2O_3 + B, or Yb + B at 1400-1500°. Hexagonal platelets. Resistant to HCl or H_2SO_4, but attacked by oxidising acids (cold HNO_3, aqua regia).

Ytterbium boride ***(YbB_{66}), 9CI*** [37322-43-3]
$B_{66}Yb$ M 886.5
Struct. contains B_{12} icosahedron surrounded by 12 B_{12}-linked icosahedra. Unit cell contains 1584 B atoms and 24 Yb atoms. Synth. from elements. Mp *ca.* 2150°. V. hard and refractory.

Post, B. *et al., J. Am. Chem. Soc.*, 1956, **78**, 1800 (*synth, struct*)
La Placa, S. *et al., Acta Crystallogr.*, 1963, **16**, 1182 (*synth, cryst struct*)
Efimova, N.I. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1788; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1559 (*synth*)
Matkovich, O.A. *et al., Zh. Neorg. Khim.*, 1968, **13**, 3155; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1627 (*synth*)
Odintsov, V.V. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, **7**, 333; *Inorg. Materials (Engl. Transl.)*, 1971, **7**, 294 (*synth, struct*)
Rea, J.R. *et al., J. Crystal Growth*, 1971, **11**, 110 (*synth, single cryst*)
Schwetz, K. *et al., J. Less-Common Met.*, 1972, **26**, 99 (*synth*)
Ames, L.L. *et al., High Temp. Sci.*, 1975, **7**, 44 (*rev*)
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Bonville, P. *et al., J. Phys. Chem. Solids*, 1978, **39**, 1273 (*mössbauer*)
Gurin, V.N. *et al., J. Less-Common Met.*, 1979, **67**, 115 (*synth, single cryst, cryst struct, electrical props*)
Aono, M. *et al., J. Phys. Chem. Solids*, 1979, **40**, 797 (*B-11 nmr*)
Golikova, O.A. *et al., J. Less-Common Met.*, 1981, **82**, 169 (*synth, electrical props*)
Iga, F. *et al., Solid State Commun.*, 1984, **50**, 903 (*synth, pe*)

[BZr]

IC-000943

Zirconium borides

[12741-10-5]

Zirconium boride ***(ZrB), 9CI, 8CI*** [12045-28-2]
Zirconium monoboride
BZr M 102.0
NaCl-type struct.

Zirconium boride ***(ZrB_2), 9CI, 8CI*** [12045-64-6]
Zirconium diboride
B_2Zr M 112.8
Hexagonal lattice with AlB_2-type struct. Synth. from elements. Employed in ceramics and as metal coatings. Mp 3050°. Attacked by HCl (1:1), H_2SO_4 (1:1) (→ H_2, SO_2, H_2S), HNO_3 (1:1); slowly by H_2O_2, or acids containing H_2O_2. Attacked also by 5-20% aq. NaOH at 80°.

Zirconium boride ***(ZrB_{12}), 9CI, 8CI*** [12046-91-2]
Zirconium dodecaboride
$B_{12}Zr$ M 220.9
Cubic lattice of UB_{12}-type struct. Synth. from elements, or B + Zr oxide at 1450-1600°. Mp *ca.* 2680°. Stable at 1500°.

Matkovich, V.I. *et al., Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1965, **122**, 116 (*cryst struct*)
Lecompasso, W.J. *et al., Mater. Res. Bull.*, 1968, **3**, 361 (*cryst struct*)
Meerson, G.A. *et al., Izv. Akad. Nauk SSSR Neorg. Mat.*, 1969, **5**, 2075; *Inorg. Materials (Engl. Transl.)*, 1969, **5**, 1787 (*pe*)
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Portnoi, K.I. *et al., Poroshk. Metall. (Kiev)*, 1970, **10**, 68; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1970, 577 (*synth, phase diagram*)
Kuzma, Yu.B. *et al., Poroshk. Metall. (Kiev)*, 1971, **11**, 51; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1971, **10**, 512 (*synth, prepn*)
Karasev, A.I., *Poroshk. Metall. (Kiev)*, 1973, **12**, 1; *Sov. Powder Metall. Met. Ceram. (Engl. Transl.)*, 1973, **12**, 777 (*manuf*)
Mavel, G. *et al., Surf. Sci.*, 1973, **35**, 109 (*pe*)
Stöhrke, M. *et al., Z. Metallk.*, 1975, **66**, 292 (*cryst struct*)
Kuzyshev, E.A. *et al., J. Less-Common Met.*, 1976, **47**, 273 (*synth, prepn*)
Boron Refract. Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
McKee, D.W., *Carbon*, 1986, **24**, 331 (*prepn*)

$B_2BaH_4O_4$

IC-000944

Barium tetrahydroxyborate

Barium metaborate tetrahydrate

[13701-59-2]

$Ba[B(OH)_4]_2$

M 295.0

Exists as several hydrates of formulation $Ba[B(OH)_4]_2.nH_2O$ or $BaO.B_2O_3.(n+2)H_2O$.

Monohydrate. [20712-54-3]. *Barium tetrahydroxyborate hydrate. Barium metaborate pentahydrate. Barium diborate pentahydrate*

$B_2BaH_{10}O_6$ M 313.0

Component of flame retardants; fungicide. Colourless cryst. Sol. H_2O. May also be formulated as $Ba(BO_2)_2.5H_2O$ or $BaO.B_2O_3.5H_2O$.

Ozols, J. *et al, Zh. Neorg. Khim.*, 1957, **2**, 2473 (*synth, monohydrate*)
Kutschabsky, L., *Acta Crystallogr., Sect. B*, 1969, **25**, 1811 (*cryst struct, monohydrate*)
Ferguson, A. *et al, Chem. Economics Handbook*, 'Boron Minerals and Chemicals', Stanford Res. Inst., USA, 1977, 717.1000A.

$B_2BaMnNa_2O_{20}Si_6Ti$ IC-000945

Tienshanite

$BaNa_2MnTiB_2Si_6O_{20}$

M 796.2

Mineral. A branched ring silicate. Occurs in a narrow vein of quartz-aegirine-microcline pegmatite of a massif in Turkestan-Alai alkalic province, southern Tienshan. Pistachio green mass. Also formulated $Na_9KCa_2Ba_6(Mn,Fe)_6(Ti,Nb,Ta)_6B_{12}[Si_{18}O_{54}]_2O_{15}(OH)_2$.

Dusmatov, V.D. *et al, Am. Mineral.*, 1968, **53**, 1426 (*mineral*)
Malinovskii, Yu.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **236**, 863; *CA*, **88**, 129285t (*cryst struct*)

$B_2BaNa_2O_{30}Si_{10}Ti_2$ IC-000946

Leucosphenite

[12360-02-0]

$Na_2BaTi_2[B_2Si_{10}O_{28}]O_2$

M 1107.5

Mineral. A branched double layer silicate. Widespread occurrence in Wyoming and Utah. Also found in Canada, Greenland and USSR. White monoclinic prisms with wedge-shaped terminations.

Pabst, A. *et al, Am. Mineral.*, 1972, **57**, 1801 (*mineral*)
Malinovskii, Yu.A. *et al, Dokl. Akad. Nauk SSSR*, 1981, **257**, 1128 (*cryst struct*)

$B_2Ba_2Ca_2FO_{28}Pb_2Si_{14}$ IC-000947

Hyalotekite, 9Cl

[12416-63-6]

$Ca_2Ba_2Pb_2B_2[(Si_{6-x}Be_{0.5})Si_6O_{28}]F$

M 1651.0

Rare mineral with a complex struct. Also formulated as $(Ba,Pb,Ca,K)_6(B,Si,Al)_2(Si,Be)_{10}O_{26}(F,Cl)$. Found in ore deposits at Långban, Sweden. Colourless or grey cryst. Forms a clear, colourless glass on heating.

Winchell, A.N. *et al, Elements of Optical Mineralogy, Part II*, 4th ed., Wiley, N.Y., 1951, 401.
Moore, P.B. *et al, Am. Mineral.*, 1982, **67**, 1012 (*cryst struct*)

$B_2Ba_4ClFe_2O_{29}Si_8Ti_2$ IC-000948

Taramellite

[61027-26-7]

$Ba_4(Fe,Ti)_4B_2[Si_4O_{12}]_2O_5Cl_2$

M 1502.5

Unbranched monocyclosilicate ($4SiO_4$ tetrahedra per unit). Mineral, occurs in limestone in Italy. Reddish-brown cryst.

Mazzi, F. *et al, Am. Mineral.*, 1980, **65**, 123 (*cryst struct*)

$B_2Ba_4ClHO_{29}Si_8Ti_2V_2$ IC-000949

Nagashimalite

[76900-97-5]

$Ba_4(V,Ti)_4B_2[Si_4O_{12}]_2O_3(O,OH)_2Cl$

M 1493.7

Unbranched monocyclosilicate (4 SiO_4 tetrahedra per unit). Mineral, found in rhodonite ore at sites in Japan. Greenish-black cryst.

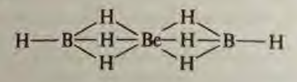
Matsubara, S., *Mineral. J.*, 1980, **10**, 131 (*cryst struct*)

B_2BeH_8 IC-000950

Bis[tetrahydroborato(1−)-*H,H'*]beryllium

Beryllium tetrahydroborate. Beryllium borohydride

[30374-53-9]



M 38.6

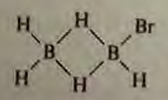
Proposed gas phase struct. shown. Chain polymer in solid state wih BeH_6 units. Synth. from $BeCl_2$ and $LiBH_4$ at 90-140°. Colourless cryst. (by subl.).

Brown, H.C. *et al, J. Am. Chem. Soc.*, 1953, **75**, 209 (*synth*)
Lipscomb, W.N. *et al, Inorg. Chem.*, 1972, **11**, 820 (*synth, struct*)
Gaines, D.F., *J. Chem. Soc., Chem. Commun.*, 1977, 224 (*gas phase nmr*)

B_2BrH_5 IC-000951

Bromodiborane(6), 8Cl

[23834-96-0]



M 106.5

Disproportionates to BBr_3 and B_2H_6. Gas. V.p. 41mm at −45°.

Stock, A., *Hydrides of Boron and Silicon*, Cornell U.P., N.Y., 1933 (*synth*)
Gaines, D.F. *et al, J. Phys. Chem.*, 1964, **68**, 955 (*pmr, B-11 nmr*)
Rietti, S.B. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 247 (*ir*)
Ferguson, A.C. *et al, J. Chem. Phys.*, 1970, **69**, 1851 (*microwave*)
Inorg. Synth., 1978, **18**, 146 (*synth, ir*)

$B_2Br_2H_4$ IC-000952

Dibromodiborane(6), 8Cl

$B_2Br_2H_4$

M 185.4

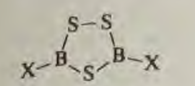
Structure unknown - probably unsymmetrical like Dichlorodiborane(6). IC-000962. Gas.

Fr. Pat., 1 480 301, (1967); *CA*, 1968, **68**, 4545 (*synth*)

$B_2Br_2S_3$ IC-000953

3,5-Dibromo-1,2,4,3,5-trithiadiborolane, 10Cl, 9Cl, 8Cl

[13863-77-9]



X = Br

M 277.6

Herbicide, fungicide and disinfectant. Liq., sensitive to moist air and reactive to many ethers, but stable to heating at 190°. Mp −17°. $Bp_{1.5}$ 50-52°, Bp_2 48°.

Schmidt, M. *et al, Angew. Chem., Int. Ed. Engl.*, 1964, **3**, 637 (*synth, props*)
Schmidt, M. *et al, Z. Anorg. Allg. Chem.*, 1966, **345**, 87 (*synth, props*)
Schmidt, M. *et al, Chem. Ber.*, 1969, **102**, 2752 (*synth, props, ir, raman*)
Sacher, R.E. *et al, J. Raman Spectrosc.*, 1973, **1**, 285 (*ir, raman*)
Zahradnik, R. *et al, Collect. Czech. Chem. Commun.*, 1974, **39**, 57 (*struct*)
Nöth, H. *et al, Chem. Ber.*, 1981, **114**, 1157; 1871 (*props, B-11 nmr, ms*)

B_2Br_4 IC-000954

Tetrabromodiborane(4), 11Cl, 10Cl, 9Cl

Boron bromide (B_2Br_4). *Diboron tetrabromide*

[14355-29-4]

$Br_2B—BBr_2$ (D_{2d})

M 341.2

Same D_{2d} (staggered) struct. persists in gas, liq. and solid phases. Clear liq., easily hydrol. Mp 0.5-1.5°.

Odom, J.D. *et al, J. Chem. Phys.*, 1972, **56**, 1643 (*ir, raman*)
Kutz, N.A. *et al, Inorg. Chem.*, 1980, **19**, 3295 (*synth, ms, B-11 nmr*)
Nöth, H. *et al, Chem. Ber.*, 1981, **114**, 398 (*synth, B-11 nmr*)
Briggs, A.G. *et al, Polyhedron*, 1984, **3**, 369 (*synth*)

B_2CaF_8 IC-000955

Calcium tetrafluoroborate(*III*)

Tetrafluoroborate(1−), calcium salt (2:1), 8Cl. Calcium fluoborate

[13814-93-2]

$Ca(BF_4)_2$

M 213.6

Synth. by either (i) passing BF_3 into Me_2CO suspensions of CaF_2 (ii) stirring toluene suspensions of CaF_2 with $BF_3.2MeOH$ or $BF_3.Et_2O$ (iii) warming CaF_2 with aq. BF_3 at 100-130°. Manuf. by reaction in an aq. medium of CaF_2, H_3BO_3 and HF. Product is dehyd. by purging with a dry inert gas (e.g. N_2) at 140-160°. Cross-linking catalyst for the polym. of epoxides and epoxy resins. Hygroscopic white powder. Dec. on heating with loss of BF_3 and formn. of CaF_2. Hydrol. in H_2O forming complex mixtures of products. V. sol. H_2O (121 g per 100 cm^3 at 20°), MeOH, Me_2CO.

de Pape, R. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1962, **254**, 4171; 1964, **259**, 3549 (*synth, dissoc*)
Pavlenko, S., *Z. Anorg. Allg. Chem.*, 1962, **315**, 136 (*synth, props*)
Marano, R.T. *et al, Therm. Anal., Proc. Int. Conf., 3rd, 1971*, 1971, **2**, 335; *CA*, 1973, **78**, 131563 (*thermal dec*)
U.S. Pat., 4 137 377, (1979); *CA*, **91**, 93787 (*manuf*)
Boiko, V.V. *et al, Zh. Prikl. Spektrosk.*, 1980, **32**, 499 (*ir*)

$B_2CaH_2MnO_6$ IC-000956

Calcium manganese borate hydrate

[12424-20-3]

$CaMn(B_2O_5).H_2O$

M 214.6

Structural studies show the composition to be $Ca_2Mn_2(OH)_4(B_4O_5(OH)_2)$. Exists as rare mineral Roweite, found in New Jersey, USA. Light brown cryst. Roweite is mod. pleochroic and is non-fluorescent.

[51846-30-1, 56645-36-4]

Macre, P.B. *et al, Am. Mineral.*, 1974, **59**, 60 (*cryst struct*)
Aristarain, L.F. *et al, Am. Mineral.*, 1974, **59**, 66 (*prop*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 84 (*rev., bibl*)

B_2CaO_4 IC-000957

Calcium metaborate (CaB_2O_4)

Calcium diborate. Boric acid (HBO_2), calcium salt, 8Cl. Calcium borate (CaB_2O_4)

[13701-64-9]

CaB_2O_4

M 125.6

One of several borates ($Ca_3B_2O_6$, $Ca_2B_2O_5$, CaB_2O_4, CaB_4O_7) formed in the $CaO—B_2O_3$ system. There are 4 polymorphs containing respectively: chains of $[BO_2]^{\ominus}$, chains of $[B_2O_4]^{2\ominus}$, a network of $[B_3O_6]^{3\ominus}$, a network of $[B_6O_{12}]^{6\ominus}$. Synth. by heating an equimolar mixture of CaO and B_2O_3 to 1200°. Colourless cryst. Mp 1162°, ΔH_f° −2192.4 kJ mol^{-1}; ΔG_f° −2084.9 kJ mol^{-1}; S° 361.1 J K^{-1} mol^{-1}.

Mineral-form

Calciborite

Struct. contains chains of $[B_2O_4]^{2\ominus}$ anions. From Ural mountains, USSR. White cryst.

Torgeson, D.R. *et al, J. Am. Chem. Soc.*, 1947, **69**, 2103 (*thermochem data*)
Kelley, K.K. *et al, J. Am. Chem. Soc.*, 1948, **70**, 1350 (*thermochem data*)
Goubeau, J. *et al, Z. Phys. Chem. (Frankfurt am Main)*, 1959, **20**, 15 (*ir, raman*)
Silver, A.H. *et al, J. Chem. Phys.*, 1960, **32**, 288 (*B-11 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 810 (*rev., bibl*)
Marezio, M. *et al, Acta Crystallogr.*, 1963, **16**, 390 (*cryst struct*)
Marezio, M. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 965 (*polymorphs, pressure*)

$B_2CaO_8Si_2$ IC-000958

Danburite

[1303-83-9]

$CaB_2(Si_2O_8)$ or $CaB_2(SiO_4)_2$

M 245.8

Framework silicate. Mineral. Rhombic, pale yellow, colourless, dark yellow, yellow-blue cryst.

Phillips, M.W. *et al, Am. Mineral.*, 1974, **59**, 79 (*cryst struct*)
Graft, M.L. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **236**, 438.
Brytov, I.A. *et al, Geokhimiya*, 1979, 281.
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)

B_2CdF_8 IC-000959

Cadmium(*II*) tetrafluoroborate

Bis(tetrafluoroborate)cadmium

[14486-19-2]

$$Cd(BF_4)_2$$

M 286.0

Obt. as solvates. Catalyst for polym. of epoxides and cross-linking; used in fluxes; battery electrode; hydrofluorination catalyst.

▷ EV0525000.

Hexahydrate: [27860-84-0]. *Hexaaquacadmium(2+) bis(tetrafluoroborate)*

From $CdCO_3$ and aq. HBF_4. Hygroscopic needles. V. sol. H_2O. Dehydration and dec. occur at 87-117°.

Heptahydrate: V. hygroscopic needles. V. sol. H_2O; spar. sol. Et_2O, EtOH.

Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1926, **155**, 327 (*hydrates*)
West, C.D., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1935, **91**, 480 (*struct, hexahydrate*)
Moss, K.C. *et al, Acta Crystallogr.*, 1961, **14**, 330 (*lattice consts, hexahydrate*)
Matsemycheva, Z.T. *et al, Zavod. Lab.*, 1964, **30**, 273 (*synth, ammine derir*)
Hague, R. *et al, Can. J. Chem.*, 1966, **44**, 2769 (*nmr*)
Ostrovskaya, T.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 338 (*synth, therm anal, hexahydrate*)
Balicheva, T.G., *Mol. Fiz. Biofiz. Vodn. Sist.*, 1973, **1**, 88; *CA*, 1974, **80**, 150623 (*ir, hexahydrate*)
Plakhotnik, V.N. *et al, Koord. Khim.*, 1978, **4**, 951 (*B-11 nmr, F-19 nmr*)

B_2CdH_8 IC-000960

Cadmium borohydride

Cadmium tetrahydridoborate. Bis[tetrahydroborato(1−)] cadmium

[43793-43-7]

$$Cd(BH_4)_2$$

M 142.0

Isolated solvates have greater thermal stability. Synth. from $CdCl_2$ and $NaBH_4$ in DMF. Reducing agent. Solid. Slow dec. in Et_2O at r.t. to Cd.

▷ Reacts violently with H_2O.

Hexaammine complex: Hexaamminecadmium bis(tetrahydroborate)

Solid.

Tris(pyridine) complex: Solid. Mp 75-76° dec.

THF complex: [37080-45-8].

Tetrakis-THF complex. Cryst. (THF at −10°). Mp 66°. Loses 3 THF at high vacuum. Dec. at 73-74°.

Wiberg, E. *et al, Z. Naturforsch., B*, 1952, **7**, 582 (*synth*)
Schenk, P.W. *et al, Chem. Ber.*, 1964, **97**, 2406 (*synth, hexaammine*)
Nöth, H. *et al, Z. Anorg. Allg. Chem.*, 1972, **389**, 225 (*synth*)

B_2ClH_5 IC-000961

Chlorodiborane(6), 11Cl, 10Cl, 9Cl, 8Cl

[17927-57-0]

M 62.1

Disproportionates to BCl_3 and B_2H_6. Colourless gas. Mp −143.6°.

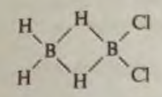
[12007-15-7]

Burg, A.B., *J. Am. Chem. Soc.*, 1934, **56**, 499 (*synth*)
Myers, H.W. *et al, Inorg. Chem.*, 1963, **2**, 655 (*synth, ir*)
Rietti, S.B. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 247 (*ir*)
Rietti, S.B. *et al, Bull. Soc. Chim. Fr.*, 1967, 2945 (*synth, ir*)
Cueilleron, J. *et al, Bull. Soc. Chim. Fr.*, 1967, 2945 (*synth, ir*)
Leach, J.B. *et al, J. Magn. Reson.*, 1972, **6**, 74 (*pmr, B-11 nmr*)
Iijima, T. *et al, Inorg. Chem.*, 1977, **16**, 3230 (*ed, gas phase struct*)
Sugie, M. *et al, J. Mol. Struct.*, 1985, **131**, 225 (*microwave*)

$B_2Cl_2H_4$ IC-000962

Dichlorodiborane(6), 11Cl, 8Cl

[12322-77-9]



M 96.5

Unsymmetrical struct. Gas.

Rietti, S.B. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 247 (*synth, ir*)
Fr. Pat., 1 480 301, (1967); *CA*, 1968, **68**, 4545 (*synth*)

$B_2Cl_2S_3$ IC-000963

3,5-Dichloro-1,2,4,3,5-trithiadiborolane, 9Cl, 8Cl

[13863-89-3]

As 3,5-Dibromo-1,2,4,3,5-trithiadiborolane, IC-000953 with

X = Cl

M 188.7

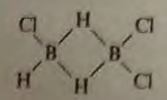
Planar molecule. Moisture-sensitive liq. Bp_{12} 66-67°.

Schmidt, M. *et al, Z. Anorg. Allg. Chem.*, 1966, **345**, 87 (*synth, props*)
Schmidt, M. *et al, Chem. Ber.*, 1969, **102**, 2752 (*ir, raman, synth*)
Almenningen, A. *et al, Acta Chem. Scand.*, 1973, **27**, 21 (*struct*)
Gropen, O. *et al, Acta Chem. Scand.*, 1973, **27**, 3079 (*props, struct*)
Sacher, R.E. *et al, J. Raman Spectrosc.*, 1973, **1**, 285 (*ir, raman*)

$B_2Cl_3H_3$ IC-000964

Trichlorodiborane(6), 11Cl

[81856-01-1]



M 131.0

Gas.

Possine, F.B.T., *Acta Sud. Am. Quim.*, 1981, **1**, 19; *CA*, 1982, **96**, 208244x (*synth, ms*)

B_2Cl_4 IC-000965

Tetrachlorodiborane(4), 11Cl, 10Cl, 9Cl

Boron chloride (B_2Cl_4), 8Cl. Diboron tetrachloride

[13701-67-2]

$$Cl_2B{-}BCl_2\ (D_{2h}\text{ or }D_{2d})$$

M 163.4

Has D_{2h} (flat) symmetry struct. in solid state but D_{2d} (staggered) in gas and liq. states. Colourless liq., easily hydrol. Mp −93°. Bp 66.5°.

Mann, D.E. *et al, J. Chem. Phys.*, 1957, **26**, 1665 (*ir, raman*)
Atoji, M. *et al, J. Chem. Phys.*, 1957, **27**, 196 (*cryst struct*)
Dibeler, V.H. *et al, Inorg. Chem.*, 1969, **8**, 50 (*ms*)
Ryan, R.R. *et al, J. Chem. Phys.*, 1969, **50**, 4986 (*ed*)
Durig, J.R. *et al, J. Chem. Phys.*, 1971, **54**, 5285 (*ir*)

Lynaugh, N. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 2192 (*pc*)
Barlos, K. *et al, Chem. Ber.*, 1977, **110**, 2774 (*B-11 nmr, Cl-35 nmr*)
Inorg. Synth., 1979, **19**, 74 (*synth*)
Briggs, A.G. *et al, Polyhedron*, 1984, **3**, 369 (*synth*)

$B_2Cl_6^{2\ominus}$ IC-000966

Hexachlorodiborate(2−)

$$[Cl_3B{-}BCl_3]^{2\ominus}$$

M 234.3 (ion)

Possible struct. shown.

Bis-tetrachlorophosphonium salt: [12297-16-4].

$B_2Cl_{14}P_2$ M 579.9

Colourless cryst. Unstable on storage, sl. volatile at −85°.

Peach, M.E. *et al, J. Chem. Soc. A*, 1968, 180 (*synth, ir*)

B_2CoF_8 IC-000967

Cobalt(*II*) tetrafluoroborate

Cobaltous fluoborate

[26490-63-1]

$$Co(BF_4)_2$$

M 232.5

Prepd. from $CoCO_3$ + aq. HBF_4. Commercially available. Red needles + $6H_2O$ (H_2O). Sol. H_2O, EtOH.

▷ GG0700000.

[15684-35-2, 37041-75-1]

Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1926, **155**, 327 (*synth*)
Moss, K.C. *et al, Acta Crystallogr.*, 1961, **14**, 330 (*cryst struct*)
Maneva, M. *et al, Monatsh. Chem.*, 1976, **107**, 337 (*ir, raman*)

$B_2CsH_5O_6$ IC-000968

Caesium tetraborate pentahydrate

[12228-83-0]

$$Cs_2B_4O_7.5H_2O$$

M 255.5

Struct. unknown; also formulated $Cs_2O.2B_2O_3.5H_2O$. Colourless solid. Mod. sol. H_2O. Loses 3 H_2O between 105-165°, and 2 between 230-400°.

Kocher, J., *Rev. Chim. Minér.*, 1966, **3**, 209 (*synth, thermal anal*)
Kocher, J., *Bull. Soc. Chim. Fr.*, 1968, 919 (*powder struct*)

B_2CuF_8 IC-000969

Copper(*II*) tetrafluoroborate

Cupric fluoborate

[38465-60-0]

$$Cu(BF_4)_2$$

M 237.1

Prepd. from CuO or $CuCO_3$ + aq. HBF_4. Commercially available. Deliquescent, blue cryst. + $6H_2O$. Sol. H_2O, EtOH.

[16455-64-8]

Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1926, **155**, 121 (*synth*)
West, C.D. *et al, Z. Kristallogr.*, 1935, **91**, 480 (*cryst struct*)

$B_2CuH_4O_6$ IC-000970

Copper metaborate dihydrate

[18851-84-8]

$$CuO.B_2O_3.2H_2O$$

M 185.1

Struct. unknown. Fungicide for wood and other cellulose based materials. Blue solid.

Svarcs, E. *et al, CA*, 1968, **68**, 6988 (*synth, thermal anal*)

B_2CuO_4 IC-000971

Copper(*II*) metaborate

Copper triborate ($Cu_3(B_3O_6)_2$)

[10290-09-2]

$$CuO.B_2O_3$$

M 149.1

Can be formulated as $[Cu_3(B_3O_6)_2]_n$. Borate anion is a 3D polymer based on 6-membered B_3O_3 rings cross-linked by addnl. bridging O. Oil pigment. Dark blue solid. Mp ~1060°.

'Trimer':

$B_6Cu_3O_{16}$ M 543.4

Martinez-Ripoli, M. *et al, Acta Crystallogr., Sect. B*, 1971, **27**, 677 (*cryst struct*)
Lecuir, L. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1971, **273**, 1091 (*synth, ir*)
Abdullaev, G.K. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1981, **22**, 637 (*cryst struct*)

$B_2Eu_2O_4$ IC-000972

Europium metaborate ($Eu_2B_2O_4$)

Europium borate oxide ($Eu_2B_2O_4$)

[38313-81-4]

$$Eu_2B_2O_4$$

M 389.5

Exists in 4 phases depending on pressure; usual struct. contains 8-coordinate Eu with infinite BO_2 chains. Isostructural with CaB_2O_4. A high pressure form has 12-coord. Eu. When 99% of $Eu^{2\oplus}$ replaced by $Sr^{2\oplus}$ v. efficient phosphor. Yellow solid (needle-like cryst.). Mp 1000°. μ_{eff} = 8.00 μ_B. Antiferromagnetic below 3K.

Hata, H. *et al, Mater. Res. Bull.*, 1977, **12**, 811.
Machida, K.-I. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 149 (*cryst struct*)
Machida, K.-I. *et al, Inorg. Chem.*, 1980, **19**, 983 (*synth, props, ir, magnetism*)

B_2F_4 IC-000973

Tetrafluorodiborane(4), 11Cl, 10Cl, 9Cl

Boron fluoride (B_2F_4), 8Cl. Diboron tetrafluoride

[13965-73-6]

$$F_2B{-}BF_2\ (D_{2h})$$

M 97.6

Struct. in solid state has D_{2h} (flat) symmetry. Latest e.d. study confirmed the gas phase struct. is D_{2h} (previously thought to be D_{2d}). Colourless gas. Mp −56°. Bp −34°.

Trefonas, L. *et al, J. Chem. Phys.*, 1958, **28**, 54 (*cryst struct at −120°*)
Brotherton, R.J. *et al, Inorg. Chem.*, 1963, **2**, 41 (*synth*)
Gales, J.N. *et al, J. Chem. Phys.*, 1964, **40**, 3516 (*synth*)
Dibeler, V.H. *et al, Inorg. Chem.*, 1968, **7**, 1742 (*ms*)
Nimon, L.A. *et al, J. Chem. Phys.*, 1970, **53**, 2416 (*ir, raman*)

Lynaugh, N. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 2192 (*pe*)
Durig, J.R. *et al, J. Chem. Phys.*, 1973, **58**, 5339 (*ir, raman*)
Barlos, K. *et al, Chem. Ber.*, 1977, **110**, 2774 (*B-11 nmr, F-19 nmr*)
Danielson, D. *et al, J. Am. Chem. Soc.*, 1977, **99**, 6484 (*ed*)

$B_2F_7^{\ominus}$ IC-000974

μ-Fluorohexafluorodiborate(1−), 11CI, 10CI, 9CI, 8CI
Heptafluorodiborate(1−)
[44801-19-6]

$[F_3B{-}F{-}BF_3]^{\ominus}$

M 154.6 (ion)
Brownstein, S. *et al, Can. J. Chem.*, 1965, **43**, 1645 (*synth*)
Harris, J.J., *Inorg. Chem.*, 1966, **5**, 1627 (*synth, ir, F-19 nmr*)
Brownstein, S., *Can. J. Chem.*, 1967, **45**, 2403 (*synth, ir*)
Hartman, J.S., *J. Chem. Soc., Chem. Commun.*, 1975, 566 (*synth, ir, F-19 nmr*)

B_2F_8Fe IC-000975

Iron(*II*) tetrafluoroborate
Ferrous fluoborate
[15283-51-9]

$Fe(BF_4)_2$

M 229.4
Prepd. from Fe + aq. HBF_4. Commercially available. V. hygroscopic, pale green needles + $6H_2O$. V. sol. H_2O, EtOH.
[13877-16-2, 15279-59-1]
Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1926, **155**, 327 (*synth*)
Moss, K.C. *et al, Acta Crystallogr.*, 1961, **14**, 330 (*cryst struct*)
Maneva, M. *et al, Monatsh. Chem.*, 1976, **107**, 337 (*ir, raman*)

B_2F_8Hg IC-000976

Mercury(*II*) tetrafluoroborate
[42921-88-0]

$Hg(BF_4)_2$

M 374.1
Prepd. in hydrated form by reaction of HgO and 40% aq. HBF_4. Used as a mercurating agent in synthesis. White, hygroscopic solid.
Barluenga, J. *et al, Synthesis*, 1979, 962 (*synth, use*)
Kumar, R. *et al, J. Organomet. Chem.*, 1987, **323**, 53 (*synth*)

B_2F_8Mg IC-000977

Magnesium tetrafluoroborate
Tetrafluoroborate(1−), magnesium salt, 8CI
[14708-13-5]

$Mg(BF_4)_2$

M 197.9
Prepd. by reaction of BF_3 and MgF_2 in C_6H_6. Commercially available in aq. soln. (30%). Creaseproofing agent for cotton fabrics. Colourless powder. Sol. H_2O.
Hexahydrate: [19585-07-0]. *Hexaaquamagnesium(2+) bis(tetrafluoroborate)*
$B_2F_8H_{12}MgO_6$ M 306.0
Cryst. from aq. solns. of $Mg(BF_4)_2$. Colourless hexagonal cryst. Formulated as $[Mg(OH_2)_6][BF_4]_2$.
Moss, K.C. *et al, Acta Crystallogr.*, 1961, **14**, 330 (*hexahydrate, cryst struct*)
de Pape, R., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1962, **254**, 4171 (*synth, props*)
Pawlenko, S. *et al, Z. Anorg. Allg. Chem.*, 1962, **315**, 136 (*thermodyn*)
Ostrovskaya, T.V. *et al, Zh. Neorg. Khim.*, 1970, **15**, 657 (*hexahydrate, thermal dec*)
Akitt, J.W., *J. Chem. Soc., Faraday Trans. 1*, 1975, **71**, 1557 (*F-19 nmr*)

B_2F_8Mn IC-000978

Manganese(*II*) tetrafluoroborate
[30744-82-2]

$Mn(BF_4)_2$

M 228.5
7-Coord. monocapped trigonal prism with one BF_4 group bridging 4 Mn atoms and one BF_4 group bridging 3 Mn atoms. Synth. from Mn powder and anhyd. HF in a rotating autoclave for 7 h. at 100-120° followed by addition of BF_3 under pressure. The mixture is then left for 31.5 h at 23°. Catalyses the alkylation of aromatic compds. with alkenes and the isom. of butane. Pink-white powder. ΔH_f −54.3 kJ mol^{-1}.
Tetrahydrate: Prepared by thermal dec. of the hexahydrate at 65-150°.
Hexahydrate: [15036-91-6]. *Hexaaquamanganese(II) tetrafluoroborate*
$B_2F_8H_{12}MnO_6$ M 336.6
Synth. from $MnCO_3$ + aq. HBF_4. Hexagonal cryst. (H_2O). Sl. sol. EtOH.
Tetrakis-MeCN complex: Synth. by treating a suspension of $NOBF_4$ in MeCN with Mn. Dec. with loss of MeCN and dec. of $BF_4^{\ominus}$ on heating.
Hexakis(MeCN) complex: Synth. from $MnBr_2$ and $AgBF_4$ in dry MeCN. Colourless cryst. (MeCN).
Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1927, **159**, 121 (*synth, hexahydrate*)
Vesely, J.A. *et al, CA*, 1959, **55**, 2596; 1963, **59**, 9988 (*synth, prop*)
Moss, K.C. *et al, Acta Crystallogr.*, 1961, **14**, 330 (*struct, hexahydrate*)
Hathaway, B.J. *et al, J. Chem. Soc.*, 1962, 2444 (*MeCN adduct*)
Pawlenko, S., *Z. Anorg. Allg. Chem.*, 1962, **315**, 136 (*thermodyn data*)
Kůtek, F., *Collect. Czech. Chem. Commun.*, 1966, **31**, 4238 (*synth, tetrahydrate*)
Libuś, W. *et al, J. Solution Chem.*, 1980, **9**, 355 (*MeCN adduct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 91; 1990, **D7**, 6 (*rev, bibl*)
Cockman, R.W. *et al, Inorg. Chem.*, 1988, **27**, 2742 (*synth, cryst struct*)

B_2F_8Ni IC-000979

Nickel(*II*) tetrafluoroborate
Nickel fluoborate
[14708-14-6]

$Ni(BF_4)_2$

M 232.2
Prepd. from $NiCO_3$ + aq. HBF_4. Commercially available. Green cryst. + $6H_2O$. Sol. H_2O, EtOH.
▷ Mod. toxic. QR6650000.
[14322-78-2, 15684-36-3]
Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1926, **155**, 327 (*synth*)
Moss, K.C. *et al, Acta Crystallogr.*, 1961, **14**, 330 (*cryst struct*)
Moneva, M. *et al, Monatsh. Chem.*, 1976, **107**, 337 (*ir, raman*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2481.

B_2F_8Pb IC-000980

Lead(*II*) tetrafluoroborate
Lead-fluoborate. Tetrafluoroborate(1−), lead(2+)(2:1), 9CI
[13814-96-5]

$Pb(BF_4)_2$

M 380.8
Prep. in aq. soln. by anodic dissoln. of Pb in HBF_4 solns. Used in electroplating baths.
▷ Toxic. ED2700000.
Rizwanul, H. *et al, Can. J. Chem.*, 1966, **44**, 2769 (*F-19 nmr*)
Chen, C.J. *et al, J. Fluorine Chem.*, 1985, **27**, 167 (*synth*)

B_2F_8Sn IC-000981

Tin(*II*) tetrafluoroborate
Tetrafluoroborate(1−), tin(2+) salt (2:1). Tin fluoborate. Stannous fluoroborate
[13814-97-6]

$Sn(BF_4)_2$

M 292.3
Prepd. in aq. soln. by anodic dissoln. of Sn in HBF_4 solns. Used to cure epoxy resins and in electroplating baths.
Rizwanul, H. *et al, Can. J. Chem.*, 1966, **44**, 2769 (*F-19 nmr*)
Chen, C.J. *et al, Electrochim. Acta*, 1985, **30**, 1307 (*synth*)

B_2F_8Zn IC-000982

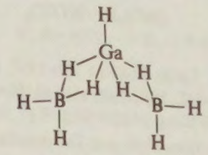
Zinc(*II*) tetrafluoroborate
Bis(tetrafluoroborato)zinc
[13826-88-5]

$Zn(BF_4)_2$

M 238.9
Forms solvates, e.g. $[Zn(NH_3)_n(BF_4)_2]$(n = 4 or 6) and $Zn(OH_2)_6(BF_4)_2$. Catalyst for crease-proofing of cotton, for polym. of epoxides, for etherification of hydroxy compds.; cross-linking catalyst; reducing agent; flame-proofing agent; component of Zn/bromine batteries; used in antistatic layers for photographic films; used in soldering fluxes.
Hexahydrate: [19585-06-9]. *Hexaaquazinc(2+) bis(tetrafluoroborate)*
Obt. by dissoln. of ZnO or $ZnCO_3$ in aq. HBF_4 soln. V. hygroscopic needles. V. sol. H_2O, EtOH. Dehydrates and dec. at 87-117°.
Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1926, **155**, 327 (*hexahydrate*)
Wilke-Dörfurst, E. *et al, Z. Anorg. Allg. Chem.*, 1927, **159**, 197 (*synth, ammine solvate*)
Ostrovskaya, T.V. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 338 (*synth, thermal anal, hexahydrate*)
Balicheva, T.G., *Mol. Fiz. Biofiz. Vodn. Sist.*, 1973, **1**, 88; *CA*, 1974, **80**, 150623 (*ir, hexahydrate*)
Gans, P. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 779 (*raman*)
Kamienska, E. *et al, Electrochim. Acta*, 1977, **22**, 181 (*conductivity*)
Libus, W. *et al, J. Solution Chem.*, 1980, **9**, 355 (*conductivity*)

B_2GaH_9 IC-000983

Hydrobis[tetrahydroborato(1−)-*H,H'*]gallium
Hydridobis(borohydrido)gallium
[61943-90-6]



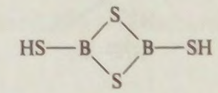
M 100.4
Synth. from $GaCl_3$ and $LiBH_4$. Thermally unstable, air- and moisture-sensitive liq. Mp *ca.* −70°. Dec. > −45°.
Downs, A.J. *et al, J. Chem. Soc., Chem. Commun.*, 1976, 825 (*synth, pmr, reactions*)
Barlow, M.T. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 597 (*ed*)

$B_2H_2S_3$ IC-000984

1,2,4,3,5-Trithiadiborolane, 9CI
[765-35-5]
As 3,5-Dibromo-1,2,4,3,5-trithiadiborolane, IC-000953 with
X = H
M 119.8
Volatile compd., sensitive to air; polymerises readily but can be stabilised as adduct with Me_3N.
Gropen, O. *et al, Acta Chem. Scand.*, 1973, **27**, 3079 (*theory*)
Zahradnik, R. *et al, Collect. Czech. Chem. Commun.*, 1974, **39**, 57 (*theory*)
Nöth, H. *et al, Z. Anorg. Allg. Chem.*, 1981, **481**, 41 (*synth, props*)

$B_2H_2S_4$ IC-000985

2,4-Dimercapto-1,3,2,4-dithiadiboretane
Metathioboric acid (dimeric form)



M 151.9
Colourless cryst. (CS_2). Sol. C_6H_6, $CHCl_3$. Mp 120°.
Wiberg, E. *et al, Z. Naturforsch., B*, 1953, **8**, 530 (*synth*)
Wiberg, E. *et al, Angew. Chem.*, 1955, **67**, 483.

B_2H_4 IC-000986

Diborane(4), 10CI, 9CI, 8CI
[18099-45-1]

$H_2B{-}BH_2$

M 25.6
Prototype of a series of compds. possessing a B—B bond; never prepd. as unsubstituted compd. in isolable state. Of theoretical interest for its unusual struct.
Armstrong, D.R., *Inorg. Chim. Acta*, 1976, **18**, 13 (*electronic struct*)
Datta, M.K. *et al, Indian J. Chem., Sect. A*, 1978, **16**, 66 (*struct*)
Bigot, B. *et al, Nouv. J. Chim.*, 1978, **2**, 449 (*struct*)
Spevacek, V. *et al, J. Mol. Struct.*, 1980, **65**, 19 (*ir*)
Vincent, M.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 5677 (*ir, struct*)

IC-000987

$B_2H_4O_4$

Hypoboric acid, 9CI

Subboric acid. Diboric acid. Tetrahydroxydiborane(4)

[13675-18-8]

$(HO)_2B—B(OH)_2$

M 89.6

Colourless solid. Loses H_2O at 100-110°, substance formed has Mp 290°. Sol. H_2O but with sl. H_2 evolution. Aq. solns. have reducing props. (e.g. $Ag^{\oplus}$ to Ag).

O,O',O'',O''' - Tetramethyl: see *Tetramethoxydiborane(4), IC-004203*

Apple, E.F. *et al, J. Am. Chem. Soc.*, 1958, **80**, 6155 (*synth*)
Nöth, H. *et al, Chem. Ber.*, 1961, **94**, 509 (*synth*)
McCloskey, A.L. *et al, J. Am. Chem. Soc.*, 1961, **83**, 4750 (*synth*)
Nikitin, V.S. *et al, CA*, 1963, **59**, 10894 (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1980, **5**, 336 (*rev, bibl*)

IC-000988

$B_2H_4O_6Zn$

Zinc diborate dihydrate

Boric acid (HBO_2), zinc salt, dihydrate, 10CI, 9CI, 8CI

[27043-84-1]

$ZnO.B_2O_3.2H_2O$

M 187.0

Commercial product; composition approximate. Used in flame retardant formulations. Colourless solid.

[51201-70-8]

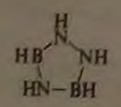
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 106 (*rev*)

IC-000989

$B_2H_5N_3$

1,2,4,3,5-Triazadiborolidine, 11CI

[333-74-4]



M 68.6

Parent member of a series of heterocyclic compds. known only in derivatised form. Of theoretical interest.

Bochvar, D.A. *et al, Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1963, 785
Boubekeur, M. *et al, Int. J. Quantum Chem.*, 1983, **23**, 891.
Boubekeur, M. *et al, Rev. Roum. Chim.*, 1984, **29**, 613.

IC-000990

$B_2H_6N_2$

Hydrazobisborane

[14809-28-0]

$[H_2B—NH=NH—BH_2]_n$

M 55.6

Polymeric. Colourless solid. Sol. dioxane, acids; stable in H_2O.

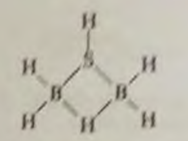
Goubeau, J. *et al, Z. Anorg. Allg. Chem.*, 1961, **310**, 123 (*synth, ir*)
Nöth, H. *et al, Adv. Chem. Ser.*, 1964, **42**, 166 (*synth*)

IC-000991

B_2H_6S

μ-Mercaptodiborane(6), 10CI, 9CI, 8CI

[22548-43-2]



M 59.7

Gas, unstable at r.t.

Keller, P.C., *Inorg. Chem.*, 1969, **8**, 2457 (*synth, ir, ms, B-11 nmr, pmr*)
Keller, P.C., *J. Chem. Soc., Chem. Commun.*, 1969, 209 (*synth, B-11 nmr*)

IC-000992

$B_2H_7^{\ominus}$

μ-Hydrohexahydrodiborate(1−), 10CI

Heptahydrodiborate(1−)

[27380-11-6]

$[H_3B—H—BH_3]^{\ominus}$

M 28.6 (ion)

Proposed to have single B—H—B bridge. Synth. from $BH_4^{\ominus}$ + B_2H_6 in CH_2Cl_2.

Tetrabutylammonium salt: [40001-25-0].
White air-sensitive cryst. Sol. CH_2Cl_2, $CHCl_3$, C_6H_6, THF.

Ph_3MeP salt: [40001-24-9].
White air-sensitive cryst. Sol. CH_2Cl_2, $CHCl_3$.

Evans, W.G. *et al, Inorg. Chem.*, 1968, **7**, 1746 (*synth*)
Inorg. Synth., 1977, **17**, 21 (*synth, pmr, B-11 nmr*)

IC-000993

$B_2H_7S^{\ominus}$

Hexahydro-μ-mercaptodiborate(1−), 8CI

$[HS(BH_3)_2]^{\ominus}$

M 60.7 (ion)

Et_4N salt: [22534-32-3].
Not isol. Sol. liq. H_2S.

Keller, P.C., *Inorg. Chem.*, 1969, **8**, 1695 (*synth, B-11 nmr*)

IC-000994

B_2H_8Mn

Manganese(*II*) borohydride

Bis(tetrahydroborato)manganese(II). Manganese(II) tetrahydroborate

$Mn(BH_4)_2$

M 84.6

Struct. not known. Synth. from $Mn(OMe)_2$ and B_2H_6 in THF or $LiBH_4$ and $MnCl_2$in dry Et_2O. Colourless compd., air-stable. Sol. Et_2O. Hydrol. slowly in H_2O but rapidly in presence of $H^{\oplus}$. Forms various THF complexes.

Monnier, G., *Ann. Chim. (Paris)*, 1957, **2**, 14 (*synth*)
Marks, T.J. *et al, Chem. Rev.*, 1977, **77**, 263 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 61 (*rev, bibl*)

IC-000995

$B_2H_8P^{\ominus}$

Hexahydro-μ-phosphidodiborate(1−), 8CI

$[H_2P(BH_3)_2]^{\ominus}$

M 60.6 (ion)

Li salt: [28961-07-1].
B_2H_8LiP M 67.6
Colourless cryst. Sol. Et_2O, H_2O. Little dec. after several hrs. in aq. soln.

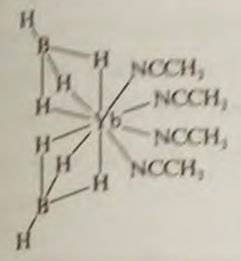
Meyer, E., *Angew. Chem., Int. Ed. Engl.*, 1971, **10**, 416 (*synth, pmr*)
Meyer, E., *Inorg. Chem.*, 1971, **10**, 2259 (*synth, ir, pmr*)

IC-000996

B_2H_8Yb

Ytterbium(*II*) borohydride

Bis(tetrahydroborato)ytterbium(II)



Tetrakis-MeCN complex

M 202.7

Eu analogue also synth.

Tetrakis-MeCN complex: [133931-87-0].
Tetrakis(acetonitrile)bis[tetrahydroborato(1−)-H,H',H'']ytterbium
$C_8H_{20}B_2N_4Yb$ M 366.9
Orange cryst. Loses 2MeCN on washing and vacuum drying; affords YbB_4 on thermal dec. at 350-400°.
Tetrakis-Py complex: [133931-89-2].
$C_{28}H_{28}B_2N_4Yb$ M 519.1
Violet cryst. + 2Py. Loses Py on washing and drying.

White, J.P. *et al, Inorg. Chem.*, 1991, **30**, 2337 (*synth, adducts, cryst struct, nmr, ir*)

IC-000997

B_2H_8Zn

Zinc tetrahydroborate ($Zn(BH_4)_2$)

Bis[tetrahydroborato(1−)]zinc. Zinc borohydride

[17611-70-0]

$Zn(BH_4)_2$

M 95.0

Obt. as Et_2O complex. Dec. at *ca.* 80°.

Mono-Et_2O complex: Synth. from MBH_4 (M = Li, Na, K) and $ZnCl_2$ in Et_2O. Selective reducing agent. Cryst. (Et_2O at −78°); removal of Et_2O leads to dec. Mp 135°.
Tetraammine complex: Tetraamminezinc(2+) bis(tetrahydridoborate)
$B_2H_{20}N_4Zn$ M 163.1
White air-stable cryst. Insol. Et_2O; dissoc. in H_2O without H_2 evolution.

Wiberg, E. *et al, Z. Naturforsch., B*, 1952, **7**, 579 (*struct*)
Nöth, H. *et al, Z. Anorg. Allg. Chem.*, 1969, **370**, 209 (*ir*)
Kedrova, N.S. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1249 (*synth, thermal anal, powder struct, ir*)
Mikheeva, V.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 225 (*synth, thermal anal, ir*)
Nakata, T. *et al, Chem. Pharm. Bull.*, 1984, **32**, 1411 (*synth, uses*)
Mal'tseva, N.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1989, **34**, 806 (*synth, ir, thermal anal, powder struct*)

IC-000998

$B_2H_{10}N_2$

μ-(Hydrazine-*N,N'*)bis(trihydridoboron)

Borane compd. with hydrazine (2:1), 9CI, 8CI. Hydrazine compd. with borane (1:2), 9CI. Hydrazine bis(borane)

[13730-91-1]

$H_3B—NH_2—NH_2—BH_3$

M 59.7

Previously considered as rocket fuel. Fine white cryst.
Does not melt below 150°.
▷ May explode violently, especially on heating. Shielding and remote-control manipulation are recommended.

Hermanek, S. *et al, Collect. Czech. Chem. Commun.*, 1966, **31**, 1281 (*chromatog*)
Inorg. Synth., 1967, **9**, 13 (*synth*)
Hanousek, F. *et al, Collect. Czech. Chem. Commun.*, 1973, **38**, 2692 (*ir, raman*)
Zakharov, V.V. *et al, Zh. Fiz. Khim.*, 1974, **48**, 499

IC-000999

$B_2H_{20}N_4Zr^{2\oplus}$

Tetraamminebis(tetrahydroborato(1−)-*H,H'*)zirconium(*IV*)(2+), 11CI

$[Zr(NH_3)_4(BH_4)_2]^{2\oplus}$

M 189.0 (ion)

8-Coordination proposed based on ir evidence.

Bis-tetrahydroborate: [84785-79-5]. *Zirconium(IV) borohydride tetraammoniate*
$B_4H_{28}N_4Zr$ M 218.7
Synth. from $Zr(BH_4)_4$ and NH_3 in toluene at −70 to −50°.

Kravchenko, O.V. *et al, Koord. Khim.*, 1982, **8**, 1650 (*synth, ir, thermal anal*)

IC-001000

$B_2I_2S_3$

3,5-Diiodo-1,2,4,3,5-trithiadiborolane, 10CI, 9CI, 8CI

[13845-20-0]

As 3,5-Dibromo-1,2,4,3,5-trithiadiborolane, IC-000953 with

X = I

M 371.6

Colourless needles, sensitive to moist air; heat stable but readily discoloured. Mp 27°. $Bp_{0.15}$ 83-85°, $Bp_{0.001}$ 35°. ^{11}B nmr δ 49.0 ppm.

Schmidt, M. *et al, Angew. Chem., Int. Ed. Engl.*, 1966, **5**, 597 (*synth, props*)
Schmidt, M. *et al, Z. Anorg. Allg. Chem.*, 1966, **345**, 87 (*synth, props*)
Schmidt, M. *et al, Chem. Ber.*, 1969, **102**, 2752 (*synth, props, B-11 nmr*)
Sacher, R.E. *et al, J. Raman Spectrosc.*, 1973, **1**, 285 (*ir, raman*)
Gates, A.S. *et al, Inorg. Chem.*, 1977, **16**, 2248 (*props*)

IC-001001

B_2I_4

Tetraiododiborane(4), 11CI, 10CI

Boron iodide (B_2I_4). Diboron tetraiodide

[13703-80-5]

$I_2B—BI_2$

M 529.2

Pale yellow solid, dec. >100°. Sol. toluene, cyclohexane. Mp 94-95°.

Haubold, W. *et al, Z. Anorg. Allg. Chem.*, 1983, **507**, 231 (*synth, ir, ms, B-11 nmr*)
Briggs, A.G. *et al, Polyhedron*, 1984, **3**, 369 (*synth*)

B_2MnS_4 IC-001002

Manganese boron sulfide (MnB_2S_4), 9CI

[50810-56-5]

MnB_2S_4

M 204.8

Orthorhombic. Prepared from the elements in an evacuated quartz tube at 1200° for 2-4 weeks. Used as a cathode in non-aq. cells with Li anode. Yellow cryst. (by subl. at 1000°).

Thomas, D. *et al*, *Bull. Soc. Chim. Fr.*, 1963, 1131 (*synth*)
Thomas, D. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1964, **258**, 2587 (*synth, struct*)
Kimmerle, F.M. *et al*, *J. Electrochem. Soc.*, 1973, **120**, 1214 (*thermochem data*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 98 (*rev, bibl*)

$B_2Mn_2O_5$ IC-001003

Manganese borate ($Mn_2B_2O_5$)

$Mn_2B_2O_5$

M 211.4

Prepd. by fusing boric acid and MnO in a Pt crucible under N_2. Orange transparent cryst. Paramagnetic-antiferromagnetic transition occurs at low temp. μ_{eff} = 5.88μ_B.

Triclinic-form

Struct. consists of $[B_2O_5]^{4\ominus}$ anions and $Mn^{2\oplus}$ cations. Cryst. (from melt). Isomorphous with $Mg_2B_2O_5$, $Fe_2B_2O_5$ and $Co_2B_2O_5$.

Monoclinic-form

Cryst. (from melt).

Monohydrate:

$B_2H_2Mn_2O_6$ M 229.5

Prepd. hydrothermally from aq. $Mn(OAc)_2$ and borax. Monoclinic struct. of composition $Mn_2(OH)[B_2O_4(OH)]$.

Mineral-form [15915-21-6]

Sussexite

$BHMnO_3$ M 114.7

Mineral identical with the monohydrate, but also sometimes formulated as $MnBO_2(OH)$. Occurs in hydrothermal veinlets at sites in USA, Switzerland and Japan. White, pinkish or straw-yellow fibrous cryst.

Block, S. *et al*, *J. Res. Natl. Bur. Stand. (U.S.)*, 1959, **62**, 95 (*struct*)
Kovalevs, L.T. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1965, **3**, 68 (*struct, ir, hydrate*)
Suknev, V.S., *J. Appl. Spectrosc. USSR (Engl. Transl.)*, 1970, **12**, 64 (*ir*)
Kovaleva, L.T. *et al*, *CA*, 1971, **75**, 113413 (*synth, hydrate*)
Park, M.J. *et al*, *Diss. Abstr. Int., B*, 1971, **31**, 7532 (*synth, B-11 nmr, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 67 (*rev, bibl*)

$B_2Mn_3O_6$ IC-001004

Manganese(*II*) borate ($Mn_3(BO_3)_2$)

$Mn_3(BO_3)_2$

M 282.4

Orthorhombic, isomorphous with $Mg_3(BO_3)_2$. Struct. consists of distorted hcp O atoms with Mn in octahedral holes. BO_3 groups cause deviation from hcp. Synth. from $MnCO_3$ and B_2O_3 (3:1 molar ratio) with a small amount of KHF_2 flux at 700° for 30 min, or by fusing MnO and boric acid in a Pt crucible under N_2. Tan cryst. μ_{eff} = 6.18μ_B.

Mineral-form [16677-55-7]

Jimboite

Manganese analogue of Kotoite. Occurs in Japan, in assoc. with carbonate ores. Light purple-brown vitreous cryst.

Watanabe, T. *et al*, *Proc. Jpn. Acad.*, 1963, **39**, 170 (*synth*)
Sadanaga, R. *et al*, *Mineral. J.*, 1964, **4**, 380 (*struct*)
Newnham, R.E. *et al*, *Phys. Status Solidi*, 1966, **16**, K17 (*magnetism*)
Suknev, V.S., *J. Appl. Spectrosc. USSR (Engl. Transl.)*, 1969, **11**, 1531 (*ir*)
Park, M.J. *et al*, *J. Korean Phys. Soc.*, 1976, **9**, 64 (*synth, B-11 nmr*)
Gaft, M.L., *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **236**, 438 (*uv-vis*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 67 (*rev, bibl*)

B_2Mn_5P IC-001005

Manganese boride phosphide (Mn_5B_2P)

Mn_5B_2P

M 327.2

Part of the Mn—P—B system. Tetragonal struct., isomorphous with Fe_5PB_2 and Mn_5SiB_2. Obt. by heating stoichiometric amounts of the elements at red heat for a few minutes and sintering *in vacuo* at 1150° for 30 h.

Rundqvist, S., *Acta Chem. Scand.*, 1962, **16**, 1 (*phase studies*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 232 (*rev, bibl*)

B_2Mn_5Si IC-001006

Manganese boride silicide (Mn_5B_2Si), 8CI

[12513-08-5]

Mn_5B_2Si

M 324.3

Isostructural with tetragonal Cr_5B_3. Obt. by arc melting of pressed samples of the elements under Ar or sintering in quartz ampoules at 900-1200°.

Aronsson, B. *et al*, *Acta Chem. Scand.*, 1960, **14**, 1403 (*synth, struct*)
Chaban, N.F. *et al*, *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 883 (*synth*)
Cely, A. *et al*, *J. Less-Common Met.*, 1978, **61**, 193 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **C8**, 355 (*rev, bibl*)

B_2NTi IC-001007

Titanium boride nitride (TiB_2N), 11CI

[52932-04-4]

TiB_2N

M 83.5

The composition is v. variable. Has fcc struct. Synth. from Ti and BN at high temp. and pressure or by chemical vapour deposition on TiN. Hard. Used as a coating on cutting tools.

[52036-95-0]

Wong, A.K. *et al*, *CA*, 1967, **66**, 86958r (*synth, use*)
Lebugle, A. *et al*, *J. Less-Common Met.*, 1981, **82**, 269 (*synth, uv-vis*)

$B_2Ni_3O_6$ IC-001008

Nickel borate ($Ni_3(BO_3)_2$)

[13850-30-7]

$Ni_3(BO_3)_2$

M 293.8

Octahedrally coord. nickel in 3-D polymeric struct. Prismatic green cryst. Insol. H_2O, acids. Isomorphous with Mn, Co analogues.

[14455-31-8]

Guyard, M.C., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1900, **130**, 335 (*synth*)
Duval, C. *et al*, *Bull. Soc. Chim. Fr.*, 1952, 101 (*ir*)
Christ, W., *Naturwissenschaften*, 1963, **50**, 567 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1966, **B3**, 772 (*rev*)
Pardo, J. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 37 (*cryst struct*)

B_2O IC-001009

Boron oxide (B_2O)

Boron suboxide

[12045-60-2]

B_2O

M 37.6

Two forms have been prepd., one with a graphite-like structure and one with a diamond-like structure.

Graphite-like-form

Formed by reducing B_2O_3 with B at ~ 6 × 10^4 atm. and 1200-1800°. Light reddish-brown solid.

Diamond-like-form

Prepd. from BP + O_2 at ~ 4 × 10^4 atm. Black-brown opaque cryst. Unreactive. V. hard. Semiconducting at 150-300K.

Hall, H.T. *et al*, *Inorg. Chem.*, 1965, **4**, 1213 (*synth, graphite-form*)
Endo, T. *et al*, *J. Mater. Sci. Lett.*, 1987, **6**, 683 (*synth, diamond-form*)

B_2O_2 IC-001010

Boron oxide (B_2O_2), 11CI, 10CI, 9CI, 8CI

Boron suboxide. Diboron dioxide

[13766-28-4]

O=B—B=O

M 53.6

Known in gas phase at high temps.

Sommer, A. *et al*, *J. Chem. Phys.*, 1963, **38**, 87 (*synth, ir*)
Demenent'ev, A.I. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1983, **24**, 252 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *3rd Suppl.*, 1987, **2**, 13 (*rev, bibl*)

B_2O_3 IC-001011

Boron oxide (B_2O_3), 11CI, 10CI, 9CI, 8CI

Diboron trioxide. Boric oxide

[1303-86-2]

B_2O_3

M 69.6

The common oxide of boron. Major use in glass manuf., also used in fibreglass, plastics and as catalyst in org. reactions and feedstock for other B compds. Commercially available. Strong Lewis acid, two crystalline forms. Hygroscopic at r.t. Bp 2250° (extrap.). ▶ RD7900000.

Hexagonal-form

Phase I. Common-form

Struct. comprises 3D network of O-bridging BO_3 groups. Used in glass technology, acid catalyst. Colourless cryst. Mp 455-475°, d 2.56 g cm^{-3}.

Orthorhombic-form

Phase II. Dense-form

Struct. comprises irregularly interconnected BO_4 tetrahedra. Obt. at 3.5 × 10^8 atm. and 525°. Mp 525-550°, d 3.11 g cm^{-3}.

Vitreous-form

Struct. prob. comprises a network of partially ordered trigonal BO_3 units with 6-membered $(BO)_3$ rings. When fused, dissolves metal oxides → coloured borate glasses. d 1.83 g cm^{-3}.

Goubeau, J. *et al*, *Z. Anorg. Allg. Chem.*, 1933, **272**, 303 (*raman*)
Dachille, F. *et al*, *J. Am. Ceram. Soc.*, 1959, **42**, 78 (*ir*)
Prewitt, C.T. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 869 (*cryst struct*)
Svansen, S.E. *et al*, *Acta Chem. Scand.*, 1969, **23**, 635 (*B-11 nmr*)
Gurr, G.E. *et al*, *Acta Crystallogr., Sect. B*, 1970, **26**, 906 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 69 (*props, use*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1980, **5**, 170 (*rev*)
Gonchar, M.A. *et al*, *CA*, 1981, **94**, 19834 (*rox*)
Windisch, C.F. *et al*, *J. Non-Cryst. Solids*, 1982, **48**, 325 (*raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *Suppl. Vol.*, 1987, **2**, 14 (*rev, bibl, use*)

$B_2O_4^{2\ominus}$ IC-001012

Diborate(2−)

$[O_2B—O—BO]_n^{2n\ominus}$

M 85.6 (ion)

Polyanion: one B atom is tetrahedral, one is trigonal planar by coordination from other $B_2O_4^{2\ominus}$ ions.

Ca salt: see *Calcium metaborate* (CaB_2O_4), *IC-000957*
Di-Ag(I) salt: Silver diborate ($Ag_2B_2O_4$)
Colourless cryst.

Shashkin, D.P. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1970, **195**, 345 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *2nd Suppl.*, 1980, **1**, 224 (*synth*)
Jansen, M. *et al*, *Naturwissenschaften*, 1980, **67**, 606 (*cryst struct*)

B_2O_4Pb IC-001013

Lead metaborate ($Pb(BO_2)_2$)

Lead borate

[14720-53-7]

$Pb(BO_2)_2$

M 292.8

Used in varnishes and paints. White crystalline powder + H_2O. Insol. H_2O, alkali, sol. acid. Loses H_2O at 160°.

[10214-39-8]

Boiko, V.F. *et al*, *Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1976, **19**, 1634, 1799.
Motoyama, M. *et al*, *Yogyo Kyokaishi*, 1977, **85**, 454 (*synth*)
Chekhovskii, V.G. *et al*, *Fiz. Khim. Steckla*, 1982, **8**, 373 (*ir*)
Kozhukharov, V. *et al*, *J. Mater. Sci.*, 1983, **18**, 1557 (*synth*)

IC-001014

$B_2O_8Zr^{6\ominus}$

Bis[orthoborato(3−)-*O*]dioxozirconate(*IV*)(6−), 11Cl

$[ZrO_2(BO_3)_2]^{6\ominus}$

M 240.8 (ion)

Tri-Mg salt: [98047-56-4]. *Magnesium zirconium borate oxide* ($Mg_3Zr(BO_3)_2O_2$)
$B_2Mg_3O_8Zr$ M 313.7
Synth. from MgO, ZrO_2 and H_3BO_3. White solid. Possesses ludwigite struct.

Konijnendijk, W.L. *et al, Mater. Chem. Phys.*, 1985, **12**, 591 (*synth, struct, luminescence*)

IC-001015

$B_2O_{10}Ti^{10\ominus}$

Bis[orthoborato(3−)-*O*]tetraoxotitanate(*IV*)(10−), 11Cl

$[TiO_4(BO_3)_2]^{10\ominus}$

M 229.4 (ion)

Penta-Mg salt: [98047-55-3]. *Magnesium titanium borate oxide* ($Mg_5Ti(BO_3)_2O_4$)
$B_2Mg_5O_{10}Ti$ M 351.0
V. efficient luminescent material. Ludwigite-like struct.

Konijnendijk, W.L. *et al, Mater. Chem. Phys.*, 1985, **12**, 591 (*synth, luminescence*)

IC-001016

B_2S_3

Boron sulfide (B_2S_3), 9Cl

[12007-33-9]

B_2S_3

M 117.8
Layer struct. composed of planar B_2S_3 6-membered rings and B_2S_2 4-membered rings linked by S bridges, B—S 181pm. Prepd. by reaction of B with H_2S or with FeS. Also by a thermal dec. of thiometaboric acid. Pale yellow solid, often glassy. Dec. in moist air. Mp 310°.
▷ Reacts violently with H_2O.

Hermann, L., *Z. Anorg. Allg. Chem.*, 1910, **66**, 362 (*synth*)
Akishin, P.A. *et al, Dokl. Akad. Nauk SSSR*, 1959, **129**, 1317 (*mol struct, gas*)
Chaplin, F. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1962, **255**, 2259 (*synth*)
Dierks, H. *et al, Angew. Chem., Int. Ed. Engl.*, 1977, **16**, 313 (*cryst struct*)
Beattie, I.R. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 267 (*ir*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 548.

IC-001017

B_2Se_3

Boron selenide (B_2Se_3), 9Cl

Boron sesquiselenide

[12297-19-7]

B_2Se_3

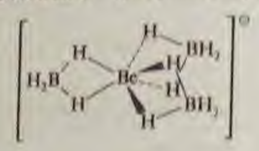
M 258.5
Prepd. by reaction of Se and B in a closed vessel or by the action of a mixt. of H_2Se and H_2 on B at 850-950°. Hygroscopic, yellow to orange amorph. powder. Extremely moisture-sensitive. Mp 479°.

Hutchinson, W.E. *et al, Inorg. Chem.*, 1962, **1**, 434 (*synth*)
Guilleron, J. *et al, Bull. Soc. Chim. Fr.*, 1967, 2973; 1972, 98 (*synth, cryst struct, thermodyn*)

IC-001018

$B_3BeH_{12}^{\ominus}$

Tris[tetrahydroborato(1−)]beryllate(1−)



M 53.5 (ion)
Proposed trigonal prismatic struct. shown.
Me_4N salt: [64933-62-6].
Synth. from $[Me_4N]BH_4$ + $Be(BH_4)_2$ for 20h at 25°. Finely divided white solid.

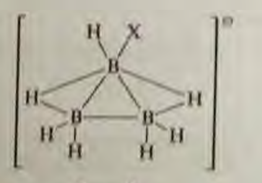
Bond, A.C. *et al, J. Am. Chem. Soc.*, 1977, **99**, 6906 (*synth, raman*)

IC-001019

$B_3BrH_7^{\ominus}$

1-Bromoheptahydrotriborate(1−), 11Cl

[94986-45-5]



X = Br

M 119.3 (ion)
Synth. from $[B_3H_8]^{\ominus}$ and Hg_2Br_2.
Tetrabutylammonium salt: [57472-92-1].
Synth. from $(Bu_4N)B_3H_8$ and HBr in CH_2Cl_2 under reduced pressure. White cryst. Dec. on heating.

[57405-81-9]

Ryschkewitsch, G.E. *et al, J. Am. Chem. Soc.*, 1975, **97**, 6258 (*synth, ir*)
Morris, J.H. *et al, Inorg. Chim. Acta*, 1982, **59**, 207 (*synth, ir, B-11 nmr*)

IC-001020

$B_3Br_3H_3N_3$

2,4,6-Tribromoborazine, 10Cl, 9Cl, 8Cl

B,B,B-Tribromoborazole

[13703-88-3]

X = Br, Y = H

M 317.1
Moisture-sensitive solid. Mp 128-129°.

Emeléus, H.J. *et al, J. Chem. Soc.*, 1939, 1306 (*synth*)
Seaife, C.W.J., *CA*, 1967, **66**, 121650h (*props*)
Heusen, K. *et al, Theor. Chim. Acta*, 1967, **9**, 17 (*nmr, uv*)
Graffeuil, M. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1971, **68**, 1379; *CA*, **76**, 19778a (*struct*)
Wrackmeyer, B. *et al, Chem. Ber.*, 1976, **109**, 3480 (*nmr*)

IC-001021

$B_3CaH_4O_8$

Dicalcium hexaborate pentahydrate

Boric acid ($H_3B_3O_3$) calcium salt (1:1) monohydrate, 8Cl

[12291-65-5]

$[Ca[B_3O_3(OH)_3].H_2O]_n$

M 205.5
Contains polymeric anion as in Hydroboracite, IC-001142. Also formulated as $2CaO.3B_2O_3.5H_2O$. Used in production of boric acid and borax. Shows interesting ferroelectric, pyroelectric and optical props. Fertiliser, fireproofing agent. Component of steel refining fluxes. Colourless monoclinic cryst. Spar. sol. H_2O; dissolves slowly in mineral acids. Dec. on heating with H_2O loss; a succession of unstable complex solid phase products are formed leading to CaB_2O_4.
▷ Explosive dehydration reaction occurs at 375°.

Mineral-form [1318-33-8]
Colemanite, 11Cl, 10Cl, 9Cl
Several formulations have been used including: $B_6H_{10}O_{11}.2Ca.5H_2O$, $B_3H_5O_7.Ca.H_2O$, $B_3H_3O_6.\frac{1}{2}Ca.H_2O$, $BHO_3.\frac{1}{4}Ca.\frac{1}{4}H_2O$, $B_2H_4O_5.2Ca.5H_2O$. Occurs in saline deposits in arid regions. Obtainable from inyoite by heating to 100°. Colourless, white or yellowish translucent cryst.

[12228-74-9, 12447-19-7, 25641-91-2, 57142-96-8, 58449-81-3]

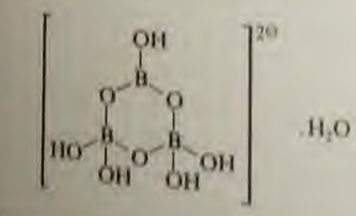
Krishnamurti, D., *Proc. - Indian Acad. Sci., Sect. A*, 1955, **41**, 7 (*vanum*)
Kamzhamov, N.A. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1990, **11**, 747 (*thermal anal*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 817 (*rev, bibl*)
Akhmanova, M.V., *Zh. Strukt. Khim.*, 1962, **3**, 28 (*ir*)
Clark, J.R. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 73 (*synth, cryst struct*)
Imamutdinova, V.M., *Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 2593 (*acid dissoln*)
Bondar, A.M., *CA*, 1972, **77**, 22769; 1981, **95**, 214251 (*ir, pmr, B-11 nmr, thermal anal*)
Thevenaz, H. *et al, Phys. Lett. A*, 1974, **49**, 218 (*B-11 nmr, ferro, pyroelectric, props*)
Filatov, S.K. *et al, CA*, 1982, **97**, 82977 (*cryst struct*)
Turner, J.B. *et al, Therm. Anal., Proc. Int. Conf., 7th, 1982*, 1982, 1, 693; *CA*, 1983, **99**, 168453 (*thermal dec*)
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)

IC-001022

$B_3CaH_5O_9$

Calcium triborate monohydrate

[37372-66-4]



M 222.5
Can also be formulated $2CaO.3B_2O_3.7H_2O$ or $Ca_2B_6O_8(OH)_4.5H_2O$. See also Calcium triborate tetrahydrate, IC-001023.

Mineral-form [1318-73-9]
Meyerhofferite, 10Cl, 9Cl
Occurs as an alteration product of inyoite in e.g. the Mt. Blanco district, California. Colourless cryst. Insol. H_2O.

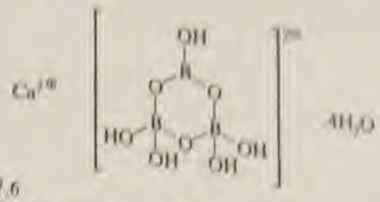
Christ, C.L. *et al, Z. Kristallogr.*, 1960, **114**, 321 (*synth*)
Clark, J.R. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 73 (*cryst struct*)
Kondrat'eva, V.V., *CA*, 1977, **88**, 25706 (*thermal anal*)

IC-001023

$B_3CaH_{12}O_{12}$

Calcium triborate tetrahydrate

[12260-25-2]



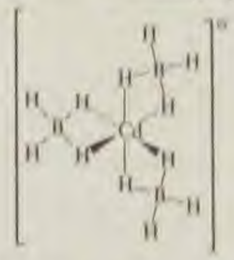
M 277.6
Can also be formulated $2CaO.3B_2O_3.13H_2O$.
Mineral-form [1318-71-4]
Inyoite, 10Cl, 9Cl
Abundant in the borate deposits of Kazakhstan, USSR and at other locations. Colourless monoclinic cryst. Mod. sol. hot H_2O.

Clark, J.R., *Acta Crystallogr.*, 1959, **12**, 162 (*synth, cryst struct*)
Christ, C.L. *et al, Z. Kristallogr.*, 1960, **114**, 321 (*synth*)
Clark, J.R., *J. Inorg. Nucl. Chem.*, 1964, **26**, 73 (*cryst struct*)
Kondrat'eva, V.V., *CA*, 1977, **88**, 25706 (*thermal anal*)
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)

IC-001024

$B_3CdH_{12}^{\ominus}$

Tris[tetrahydroborato(1−)]cadmate(1−)



M 156.9 (ion)
From $CdCl_2$ and MBH_4 in Et_2O or THF.
Li salt: [37080-50-5]
Solid.
Na salt: [37080-49-2]
Solid.

Nöth, H. *et al, Z. Anorg. Allg. Chem.*, 1972, **389**, 225 (*synth*)

IC-001025

B_3CeH_{12}

Cerium(*III*) borohydride

Tris[tetrahydoborato(1−)-H,H']cerium(III), 10Cl

[83618-19-3]

$Ce(BH_4)_3$

M 184.6
Air and moisture-sensitive solid. Generally obt. as THF solvate.

Tris-THF solvate. Tris(tetrahydroborato) tris(tetrahydrofuran)cerium(III)
$C_{12}H_{36}B_3CeO_3$ M 400.9
Air and moisture-sensitive cryst. Sol. C_6H_6, THF. Mp 253° dec. Desolvates at 100-110°.

[83618-22-8]

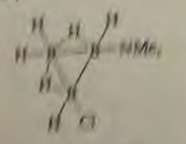
Mirsaidov, U. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 1722; *Inorg. Materials (Engl. Transl.)*, 1979, **15**, 1560 (*synth*)

Kravchenko, O.V. et al. Russ. Khim. 1980, 5, 76, 1030. Alexandrov, U. et al. Zh. Neorg. Khim., 1981, 27, 2436; Russ. J. Inorg. Chem. (Engl. Transl.), 1982, 27, 1378 (synth, IR)

IC-001028

B_2CH_5

Chloroditetraborane(7)



NMe_3 complex

M 73.9
Obtd. as complexes
Me_3N complex: [99165-86-2]
$C_5H_{14}B_2ClN$ M 133.0
Sol. CH_2Cl_2, $CHCl_3$
Me_3P complex: [129916-78-5]. *1-Chloro-3-(trimethylphosphine)triborane(7), 1ICl*
$C_4H_{14}B_2ClP$ M 150.0
Toeddo, A.R. et al. Inorg. Chem., 1990, 29, 4617 (synth, pmr, B-11 nmr, ms)

B_2CH_7O **IC-001027**

1-Chloroheptahydrotriborate(1−)

[37968-04-3]

As 1-Bromoheptahydrotriborate(1−), IC-001019 with

X = Cl

M 94.9 (ion)
Synth. from $[B_3H_8]^\ominus$ and $HgCl_2$ as r.t.
Tetrabutylammonium salt: [57670-09-4].
White cryst.
Bis(triphenylphosphine)iminium salt: [82383-88-8].
White cryst.

Morris, J.H. et al, Inorg. Chim. Acta, 1982, 59, 207 (synth, ir, B-11 nmr)
Morris, J.H. et al, J. Chem. Soc., Dalton Trans., 1984, 2525 (synth)

$B_2ClO_{10}Pb_4$ **IC-001028**

Lead borate chloride oxide ($Pb_4(BO_2)_2ClO$), 1ICl

[87754-78-7]

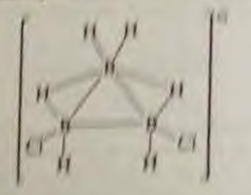
$Pb_4O[Pb_2(BO_2)_2Cl]$

M 1471.6
Orthorhombic. Struct. composed of Pb_4O tetrahedra, Pb—Pb units, planar BO_2 groups and isolated $Cl^\ominus$ ions. Synth. from melt of PbO, $PbCl_2$ and H_3BO_3. Rod shaped cryst.

Behm, H., Acta Crystallogr., Sect. C, 1983, 39, 1317 (cryst struct)

$B_2Cl_2H_5^\oplus$ **IC-001029**

1,2-Dichlorohexahydrotriborate(1+), 1ICl



M 109.3 (ion)
Synth. from $[B_3H_8]^\ominus$ and $2HgCl_2$ or from $[B_3H_8]^\ominus$ in CH_2Cl_2 with HCl gas.
Tetrabutylammonium salt: White cryst.
Bis(triphenylphosphine)iminium salt: [94986-37-5]. Colourless cryst. (CH_2Cl_2/hexane).

Morris, J.H. et al, Inorg. Chim. Acta, 1982, 59, 207; 1984, 103, 31 (pmr, synth, ir, B-11 nmr)
Morris, J.H. et al, J. Chem. Soc., Dalton Trans., 1984, 2531 (synth, struct, electrochem, B-11 nmr)
Morris, J.H. et al, Polyhedron, 1986, 5, 1639 (B-11 nmr)

$B_3Cl_3H_3N_3$ **IC-001030**

2,4,6-Trichloroborazine, 10Cl, 9Cl, 8Cl

B,B,B-Trichloroborazole

[933-18-6]

As 2,4,6-Tribromoborazine, IC-001020 with

X = Cl, Y = H

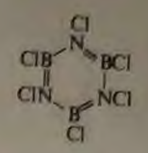
M 183.8
Curing agent for epoxy resins. Colourless orthorhombic cryst. slowly dec. under N_2 at 0°; sublimes readily; moisture sensitive. Sol. C_6H_6, CCl_4, Et_2O, CS_2, PhCl, cyclohexane, $CHCl_3$, insol. Py, $PhNO_2$. d_4^{25} 1.58. Vigorous reaction with H_2O and alcohols. Above 100° slow irreversible dec. occurs with formation of HCl.

Brown, C.A. et al, J. Am. Chem. Soc., 1955, 77, 3699 (synth, props)
Brennan, G.L. et al, J. Am. Chem. Soc., 1960, 82, 6248 (props)
Inorg. Synth., 1972, 13, 41 (synth, props, ir, pmr)
Kroner, J. et al, Tetrahedron, 1972, 28, 1585 (pe)
Melcher, L.A. et al, Inorg. Chem., 1973, 12, 601 (ms)
Wrackmeyer, B. et al, Chem. Ber., 1976, 109, 3480 (nmr)
Molt, K. et al, Z. Anorg. Allg. Chem., 1981, 474, 182 (ir, raman)

$B_3Cl_6N_3$ **IC-001031**

Hexachloroborazine, 9Cl

[19087-72-0]



M 287.1
Prepd. from NCl_3 + BCl_3 in CCl_4 at <45°. Cryst. (CCl_4). V. reactive towards nucleophilic reagents. Mp 187°. Bp 250-260° dec.

Haasnoot, J.G. et al, Inorg. Nucl. Chem. Lett., 1967, 3, 597 (synth)
Haasnoot, J.G. et al, Acta Crystallogr., Sect. B, 1972, 28, 2070 (cryst struct)
Gopinathan, M.S. et al, Acta Crystallogr., Sect. B, 1974, 30, 731 (cryst struct)

IC-001032

B_3DyH_{12}

Dysprosium(III) borohydride

Tris[tetrahydroborato(1−)-H,H']dysprosium(III), 10Cl

[68647-97-8]

$Dy(BH_4)_3$

M 201.6
Obtd. as THF complex.
Tris-THF complex: [71856-55-8]. *Tris(tetrahydroborato) tris(tetrahydrofuran)dysprosium(III)*
$C_{12}H_{36}B_3DyO_3$ M 423.3
Yellow-white cryst. Sol. THF.

Zange, E., Chem. Ber., 1960, 93, 652 (synth)
Mirsaidov, U. et al, Zh. Neorg. Khim., 1978, 23, 3326; Russ. J. Inorg. Chem. (Engl. Transl.), 1978, 23, 1845 (synth)
Mirsaidov, U. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1979, 15, 1585; Inorg. Materials (Engl. Transl.), 1979, 15, 1248 (synth)

IC-001033

B_3ErH_{12}

Erbium(III) borohydride

Tris[tetrahydroborato(1−)-H,H']erbium(III), 9Cl

$Er(BH_4)_3$

M 211.7
Generally obtd. as THF complex.
Bis-THF complex:
$C_{10}H_{28}B_3ErO_2$ M 356.0
Hygroscopic pink powder. Desolvated at 100° with some loss of H_2.
Tris-THF solvate: [57485-17-3]. *Tris(tetrahydroborato) tris(tetrahydrofuran)erbium(III)*
$C_{16}H_{44}B_3ErO_3$ M 428.1
Rose-coloured cryst. $\mu_{eff} = 8.83\mu_B$ (high temps.); $\mu_{eff} = 5.16\mu_B$ (low temps.).

Zange, E., Chem. Ber., 1960, 93, 652 (synth)
Bernstein, E.R. et al, Chem. Phys., 1975, 10, 215 (synth, us)
Mirsaidov, U. et al, Zh. Neorg. Khim., 1977, 22, 2862; 1978, 23, 931; Russ. J. Inorg. Chem. (Engl. Transl.), 1977, 22, 1555; 1978, 23, 1062 (synth, ir)

B_3EuH_{12} **IC-001034**

Europium(III) borohydride

Tris[tetrahydroborato(1−)-H,H']europium(III), 9Cl

[74463-08-4]

$Eu(BH_4)_3$

M 196.4
Pale yellow-green cryst. Sol. THF. Tetra, hexa and octa-THF solvates reported.

Zange, E., Chem. Ber., 1960, 93, 653 (synth)
Mirsaidov, U. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1978, 14, 1722 (synth)
Mirsaidov, U. et al, Zh. Neorg. Khim., 1980, 25, 1620; Russ. J. Inorg. Chem. (Engl. Transl.), 25, 899 (synth)

$B_3F_3H_3N_3$ **IC-001035**

2,4,6-Trifluoroborazine, 10Cl, 9Cl, 8Cl

B-Trifluoroborazine

[13779-24-3]

As 2,4,6-Tribromoborazine, IC-001020 with

X = F, Y = H

M 134.4

White cryst. Sol. Et_2O, C_6H_6, CCl_4, CS_2, toluene, oxyl- and cyclohexane, pet. ether. Solid in vacuo. Reacts with moist air.

Nicholson, B., Inorg. Chem., 1965, 4, 983 (synth)
Lindemayer, R.W. et al, Inorg. Chem., 1967, 6, 519 (r, str, soln)
Kroner, J. et al, Tetrahedron, 1973, 29, 1585 (pe)
Melcher, L.A. et al, Inorg. Chem., 1973, 12, 601 (mss)
Wrackmeyer, B. et al, Chem. Ber., 1976, 109, 3480 (nmr)
Molt, K. et al, Z. Anorg. Allg. Chem., 1981, 474, 182 (ir)

B_3F_5

Boron fluoride (B_3F_5), 8Cl **IC-001036**

Triboron pentafluoride

[15538-67-7]

$FB(BF_2)_2$

M 127.4
Unstable in gas phase. Dec. at −95° in a few hrs.

Timms, P.L., J. Am. Chem. Soc., 1967, 89, 1629 (synth, fi, ms, F-19 nmr)

$B_3F_{10}^\ominus$ **IC-001037**

Decafluorotriborate(1−)

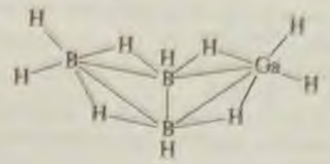
$[F_2B—F—BF_2—F—BF_2]^\ominus$

M 222.4 (ion)
Stable only at low temps.
Ag salt:
AgB_3F_{10} M 330.2
Stable between −90 and −60°. Sol. CH_2Cl_2.
Tetrabutylammonium salt: Stable between −90 and −35°.

Brownstein, S. et al, Can. J. Chem., 1965, 43, 1645 (synth, F-19 nmr)

B_3GaH_{10} **IC-001038**

2-Gallatetraborane(10)



M 112.2
arachno-. Synth. from $(Bu_4N)B_3H_8$ and $GaClH_2$ at −30°. Colourless liq. Sol. toluene. Mp *ca.* −95°. V. p. *ca.* 1 mm at −63°. Dec. >10° to Ga, H_2, B_4H_{10}; vapour dec. to GaB_3, B_2H_6 + H_2.

Pulham, C.R. et al, J. Chem. Soc., Chem. Commun., 1990, 1520 (synth, ir, pmr, B-11 nmr, ms, ed, struct)
Duke, B.J., J. Chem. Soc., Chem. Commun., 1991, 123 (theory)

B_3GdH_{12} **IC-001039**

Gadolinium(III) borohydride

Tris(tetrahydroborato)gadolinium(III)

$Gd(BH_4)_3$

M 201.7
Obtd. as THF complex.
Tris-THF complex:
$C_{12}H_{36}B_3GdO_3$ M 418.0

$B_3H_2Na_3O_7 - B_3H_6N_3$

Air- and moisture-sensitive colourless cryst. Isomorphous with Y analogue, Yttrium(*III*) borohydride, IC-001061

Bernstein, E.R. *et al*, *Chem. Phys.*, 1975, **10**, 215 (*synth*)
Segal, B.G. *et al*, *Inorg. Chem.*, 1978, **17**, 844 (*cryst struct*)

IC-001040

$B_3H_2Na_3O_7$

Sodium metaborate hemihydrate

Trisodium triborate

[56831-57-9]

$NaBO_2.\frac{1}{2}H_2O$ (struct. unknown)

M 215.4

It has been suggested that this compd. is $Na_2[B_3O_3(OH)_4]$.

Colourless orthorhombic cryst.

Nies, N.P. *et al*, *J. Chem. Eng. Data*, 1967, **12**, 303 (*synth*)
Tolstikova, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **271**, 1577 (*thermal anal*)
Corazza, E. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1983 (*formulation*)
Nies, N.P., *Mellor Compr. Treat. Inorg. Theor. Chem.*, Longman, London, 1980, **V/A**, 361 (*rev*)

IC-001041

$B_3H_3S_3$

Thioboric acid ($H_3B_3S_3$), 10Cl, 9Cl, 8Cl

Monothioboric acid. Thioborazine. 2,4,6-Trimercapto-cyclo-1,3,5-triaza-2,4,6-triborine. Trimercaptoborazine

[13703-87-4]

M 177.9

Colourless cryst. (CS_2). Sol. CS_2, C_6H_6, CCl_4, $CHCl_3$. Mp 160° dec.

S,S',S''-Trimethyl 2,4,6-*Trimercaptoborazine*

$C_6H_9B_3S_3$ M 266.4

Tri-Na salt [23361-58-2]

B_3NaS_3 M 201.7

Synth. as tri-K salt with Na_2S. V. moisture-sensitive, highly unstable. Mp 580°. Isostructural with corresp. morpholide.

Tri-K salt [23361-56-0]

B_3KS_3 M 342.1

Synth. from B,S, and K,S in a sealed tube at 700° or action of H_2S in an excess of N_2 on K,S and B at 750°. V. moisture-sensitive highly unstable. Mp 530° Isostructural with corresp. morpholide.

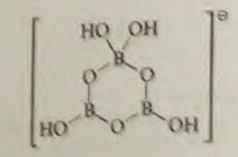
Wiberg, E. *et al*, *Z. Naturforsch., B*, 1953, **8**, 532 (*synth*)
Edwards, J.O. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 2037 (*rev*)
Clemens, D. *et al*, *J. Mol. Struct.*, 1969, **3**, 57 (*cr. X-ray solid*)
Schwarz, W. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 2029 (*cryst struct*)
Hilal, R. *et al*, *Bull. Soc. Chim. Fr.*, 1974, 85 (*IR-11 spec*)
Gates, A.S. *et al*, *Inorg. Chem.*, 1977, **16**, 2240 (*rv. refrnce*)

IC-001042

$B_3H_4O_7^{\ominus}$

Triborate(1−)

[12344-77-3]



M 148.4 (ion)

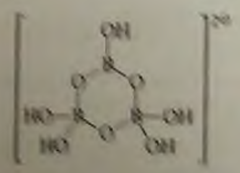
K salt: [12271-94-2]. *Potassium triborate* ($KH_4B_3O_7$)
$B_3H_4KO_7$ M 187.5
Colourless cryst. Sol. H_2O (reacts slowly). Better formulated as $K[B_3O_3(OH)_4].H_2O$. Loses H_2O between 100-550° to give KB_3O_5.

Ingo, N., *Acta Chem. Scand.*, 1963, **17**, 573, 581 (*synth*)
Heller, G., *J. Inorg. Nucl. Chem.*, 1967, **29**, 2181 (*synth*)
Dal Negro, A. *et al*, *Am. Mineral.*, 1975, **60**, 879 (*cryst struct*)
Miseda, M. *et al*, *J. Inorg. Nucl. Chem.*, 1979, **41**, 1217 (*raman*)
Jandn, R. *et al*, *Z. Naturforsch., B*, 1979, **34**, 585 (*ir*)
Salentine, C.G., *Inorg. Chem.*, 1983, **22**, 3920; 1987, **26**, 128 (*synth, ir, raman, cryst struct, B-11 nmr*)

IC-001043

$B_3H_4O_9^{3\ominus}$

Triborate(2−)



M 185.4 (ion)

Mg salt: see *Magnesium triborate pentahydrate*, IC-001064
Ca salt: see *Calcium triborate monohydrate*, IC-001022
Cu salt: see *Calcium triborate tetrahydrate*, IC-001025
Zn salt: see *Zinc triborate monohydrate*, IC-001047
Trimm, D.L. *et al*, *J. Magn. Reson.*, 1969, **67**, 544 (*B-11 nmr*)

IC-001044

$B_3H_6N_3$

Borazine, 10Cl, 9Cl

Trimeric(cyclic)borane. Borazole. Hexahydro-s-triazatriborine

[6569-51-3]

R = R' = H

M 80.5

Inorganic benzene analogue. Liq. d^{25} 0.808. Mp −58°. Bp 55°. n_D^{20} 1.3821. Dipole moment 0.58D. Dec. slowly at r.t. to give hydrogen and a nonvolatile residue. Hydrol. slowly in water to $B(OH)_3$.

2,4,6-Tri-Me: see *2,4,6-Trimethylborazine*, IC-005720
Hexa-Me: see *Hexamethylborazine*, IC-005304
2,4,6-Tri-Et: see *2,4,6-Triethylborazine*, IC-005305
2,4,6-Tri-Ph: see *2,4,6-Triphenylborazine*, IC-005003
Stock, A. *et al*, *Ber.*, 1926, **59**, 2215 (*synth*)
Schaeffer, R. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 3303 (*synth*)

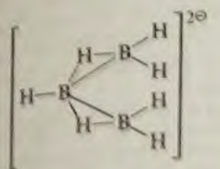
Nielsen, W.S. *et al*, *Inorg. Chem.*, 1967, **6**, 1453 (*ir, raman*)
Hamilton, W. *et al*, *Inorg. Chem.*, 1969, **8**, 1683 (*cryst struct*)
Porter, R.F. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 56 (*ms*)
Wrackmeyer, B. *et al*, *Chem. Ber.*, 1976, **109**, 3480 (*nmr*)

IC-001045

$B_3H_7^{2\ominus}$

Heptahydrotriborate(2−)

[13429-71-9]



possible structure

M 19.4 (ion)

Not generally recognised as a stable anion. Known only as ligand e.g. $(CO)_9Fe_2B_3H_7$; $(Me_2PPh)_2PtB_3H_7$.

Kasle, S.F.A. *et al*, *J. Chem. Soc. A*, 1969, 2007 (*theory*)
Kennedy, J.D., *Prog. Inorg. Chem.*, 1984, **32**, 519.

IC-001046

B_3H_7

Triborane(7), 11Cl, 10Cl, 9Cl, 8Cl

[12029-70-8]

M 39.4

Unstable - Struct. shown is probable struct. of most stable form.

thf complex: [12347-17-0]. *Triborane(7) compd. with methyl ether (1:1)*
$C_5H_{15}BO$ M 85.5
Mp 10.5-11.1°.

PH3 complex: see *Triborane(7) compd. with phosphine (1:1)*, IC-001049

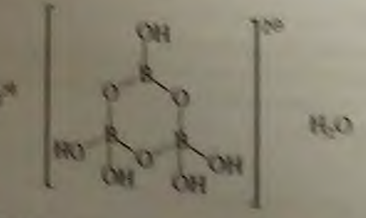
Onak, W.S. *et al*, *Inorg. Chem.*, 1968, **7**, 1038 (*synth*)
Calabro, G., *Inorg. Chem.*, 1975, **14**, 452 (*B-11 nmr*)
Bishop, V.L. *et al*, *Inorg. Chem.*, 1981, **20**, 2724 (*synth, proc, B-11 nmr, X-ray nmr*)
Simons, J.P. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 5885 (*theory*)

IC-001047

$B_6O_{13}Zn$

Zinc triborate monohydrate, 10Cl, 9Cl

[1329-75-1]



M 306.8

Can be formulated as shown or as $2ZnO.3B_2O_3.7H_2O$.

Commercially available. Fire-retardant additive in plastics. Colourless solid. Spar. sol. H_2O.

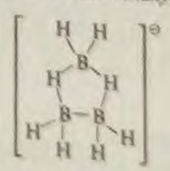
Lehmann, H.A. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **354**, 37 (*synth, ir*)
Ozols, J.K. *et al*, *CA*, 1973, **78**, 165580; *CA*, 1979, **90**, 130736 (*synth, cryst struct*)

IC-001048

$B_3H_8^{\ominus}$

Octahydrotriborate(1−), 10Cl

Triborohydride(1−). Di-μ-hydrohexahydrotriborate(1−)



M 40.4 (ion)

arachno-anion.

Tetrabutylammonium salt: [53451-55-1].
$C_{16}H_{44}B_3N$ M 282.9
Used in synth. of higher boranes, borane anions, carboranes and transition metal complexes. White cryst. (CH_2Cl_2/Et_2O), stable to air and water. Sol. CH_2Cl_2, MeCN, spar. sol. C_6H_6, Et_2O, hexane, H_2O.

Inorg. Synth., 1974, **15**, 113 (*synth, struct*)

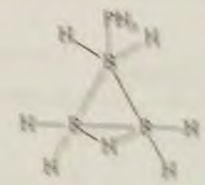
IC-001049

$B_3H_{10}P$

Triborane(7) compd. with phosphine (1:1), 10Cl

Phosphine triborane(7)

[77589-49-2]



M 73.4

Air-sensitive colourless liq. Sol. CH_2Cl_2.

Bishop, V.L. *et al*, *Inorg. Chem.*, 1981, **20**, 2724 (*synth, rea, proc, B-11 nmr, X-ray nmr*)

IC-001050

$B_6H_{12}Ho$

Holmium(III) borohydride

Tris[tetrahydroborato(1−)-H,H']holmium(III), 10Cl

[72804-73-4]

$Ho(BH_4)_3$

M 208.4

Obtd. as THF solvate.

Tris-THF solvate [71898-57-8]. *Tris(tetrahydroborato-tris(tetrahydrofuran)holmium(III)*
$C_{12}H_{36}B_3HoO_3$ M 425.7
Amber coloured cryst. Sol. THF

[73204-51-5]

Mirsaidov, U. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1979, **15**, 1585; *Inorg. Mater.(Engl. Transl.)*, 1979, **15**, 1240 (*synth*)

IC-001051

$B_3H_{12}La$

Lanthanum(III) borohydride

Tris[tetrahydroborato(1−)-H,H']lanthanum(III)

$La(BH_4)_3$

M 183.4

Air- and moisture-sensitive white solid. Mp 261° dec. Usually obt. as THF solvate.

Tris-THF complex: [103173-13-3].
Air- and moisture-sensitive colourless cryst. Sol. C_6H_6, toluene. Desolvates >100-110°. Isomorphous with Gd, Y analgues.

Bernstein, E.R. *et al, Chem. Phys.*, 1975, **10**, 215 (*synth*)
Kravchenko, O.V. *et al, Koord. Khim.*, 1980, **6**, 76; **6**, 1030.
Mirsaidov, U. *et al, Zh. Neorg. Khim.*, 1982, **27**, 2436; 1986, **31**, 1321; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 1376; 1986, **31**, 753 (*synth, ir*)

$B_3H_{12}Lu$ IC-001052

Lutetium(*III*) borohydride

Tris[tetrahydroborato(1−)-H,H′]lutetium(III), *10CI*

[71722-78-6]

$Lu(BH_4)_3$

M 219.4
Obtd. as THF solvate.

Tris-THF solvate: [103173-14-4]. *Tris(tetrahydroborato) tris(tetrahydrofuran)lutetium*(III)
$C_{12}H_{36}B_3LuO_3$ M 435.8
Air-sensitive colourless cryst. Sol. THF. Isomorphous with Gd, Y analogues.

[81809-37-2]

Mirsaidov, U. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **15**, 1585; *Inorg. Materials (Engl. Transl.)*, 1978, **15**, 1248 (*synth*)
Mirsaidov, U. *et al, Zh. Neorg. Khim.*, 1986, **31**, 1321; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1986, **31**, 753 (*synth, cryst struct*)

$B_3H_{12}Nd$ IC-001053

Neodymium(*III*) borohydride

Tris[tetrahydroborato(1−)-H,H′]neodymium(III), *9CI*

$Nd(BH_4)_3$

M 188.7
Obt. as THF complex.

Tris-THF complex: [103194-52-1]. *Tris(tetrahydroborato) tris(tetrahydrofuran)neodymium*(III)
$C_{12}H_{36}B_3NdO_3$ M 405.0
Light blue needles. Sol. THF. Mp 161-163°. Isomorphous with Gd, Y analogues.

[69942-17-2]

Bernstein, E.R. *et al, Chem. Phys.*, 1975, **10**, 215 (*synth*)
Andersen, R.A., *Inorg. Chem.*, 1979, **18**, 1507 (*synth, ir*)
Makhaev, V.D. *et al, Zh. Neorg. Khim.*, 1981, **26**, 45; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 1417 (*synth, use*)
Mirsaidov, U. *et al, Zh. Neorg. Khim.*, 1986, **31**, 1321; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1986, **31**, 753 (*synth, cryst struct*)

$B_3H_{12}Pr$ IC-001054

Praseodymium(*III*) borohydride

Tris[tetrahydroborato(1−)]praseodymium(III)

[68929-25-9]

$Pr(BH_4)_3$

M 185.4
Obt. as THF solvate.

Tris-THF solvate: [100198-50-3].
Air- and moisture-sensitive cryst. Sol. THF.

Mirsaidov, U. *et al, Zh. Neorg. Khim.*, 1978, **14**, 1722; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **14**, 1340 (*synth*)

$B_3H_{12}Sc$ IC-001055

Scandium(*III*) borohydride

Tris(tetrahydroborato)scandium(III)

$Sc(BH_4)_3$

M 89.4

Bis-THF complex: [63312-92-5].
Air-sensitive colourless cryst. Sol. C_6H_6. Subl.$_{0.001}$ 100°. Cryst struct. shows two BH_4 triply bridged, one bonded via 2H. Other THF complexes also claimed.

Morris, J.H. *et al, J. Chem. Soc., Chem. Commun.*, 1970, 245 (*synth, ms, raman, ir*)
Lobkovskii, E.B. *et al, Zh. Strukt. Khim.*, 1977, **18**, 389; *J. Struct. Chem. USSR (Engl. Transl.)*, 1977, **18**, 312 (*cryst struct*)
Mirsaidov, V. *et al, Zh. Neorg. Khim.*, 1980, **25**, 1386; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 769 (*synth*)
Mancini, M. *et al, Inorg. Chem.*, 1984, **23**, 1072 (*Sc-45 nmr, pmr, ir*)

$B_3H_{12}Sm$ IC-001056

Samarium(*III*) borohydride

Tris[tetrahydroborato(1−)-H,H′]samarium(III), *10CI*

[68929-26-0]

$Sm(BH_4)_3$

M 194.8
Solid. Sol. THF.

Tris-THF complex: [79845-87-7].
Air- and moisture-sensitive cryst. Sol. THF. Tetra-THF and octa-THF solvates also reported.

Zange, E., *Chem. Ber.*, 1960, **93**, 652 (*synth*)
Mirsaidov, U. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 722 (*synth*)
Mirsaidov, U. *et al, Zh. Neorg. Khim.*, 1980, **25**, 1620; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 899 (*synth, dta*)

$B_3H_{12}Tb$ IC-001057

Terbium(*III*) borohydride

Tris[tetrahydroborato(1−)-H,H′]terbium(III), *10CI*

$Tb(BH_4)_3$

M 203.4
Obtd. as THF solvate.

Tris-THF solvate: [71911-21-2]. *Tris(tetrahydroborato) tris(tetrahydrofuran)terbium*
$C_{12}H_{36}B_3O_3Tb$ M 419.7
Air- and moisture-sensitive white solid. Sol. THF.

Zange, E., *Chem. Ber.*, 1960, **93**, 652.
Mirsaidov, U. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1979, **15**, 1585; *Inorg. Materials (Engl. Transl.)*, 1979, **15**, 1248 (*synth*)

$B_3H_{12}Ti$ IC-001058

Titanium(*III*) borohydride

Tris(borohydrido)titanium(III). *Tris[tetrahydroborato(1−)-H,H′,H″]titanium*(III), *11CI*. *Titanium tris(tetrahydroborate)*

[82248-53-1]

$Ti(BH_4)_3$

M 92.4
Thought to have distorted O_h geometry in solid state, with bidentate BH_4, but tridentate in gas phase with C_{3v} symmetry. Synth. by grinding $TiCl_4$ + $LiBH_4$ in a vacuum vibration mill. Catalyses ethylene polym. when adsorbed on SiO_2 or Al_2O_3 surfaces. Dec. >20°, forming TiB_2.

[62387-90-0]

Volkov, V.V. *et al, Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1977, 77; *CA*, **86**, 132712u (*synth, ir*)
Nesterov, G.A. *et al, Vysokomol. Soedin., Ser. B*, 1979, **21**, 755; *CA*, **92**, 22903y (*use*)
Davis, C.J. *et al, Angew. Chem.*, 1982, **94**, 557 (*synth, ed*)

$B_3H_{12}Tm$ IC-001059

Thulium(*III*) borohydride

Tris(tetrahydroborato(1−)-H,H′]thulium(III), *10CI*

[71722-77-5]

$Tm(BH_4)_3$

M 213.4
Obtd. as THF solvate.

Tris-THF solvate: [71896-58-7]. *Tris(tetrahydroborato) tris(tetrahydrofuran)thulium*(III)
$C_{12}H_{36}B_3O_3Tm$ M 429.7
Dark green cryst. Sol. THF.

Mirsaidov, U. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1979, **15**, 1585; *Inorg. Materials (Engl. Transl.)*, 1979, **15**, 1248 (*synth*)

$B_3H_{12}U$ IC-001060

Uranium(*III*) borohydride

Uranium tris(tetrahydroborate). Tris[tetrahydroborato(1−)] uranium(III)

[65579-07-9]

$U(BH_4)_3$

M 282.5
Formed by thermal dec. of $U(BH_4)_4$ at 127°. Red-brown solid.

▷ Pyrophoric.

Tris-THF complex: [102695-65-8]. *Tris(tetrahydroborato) tris(tetrahydrofuran)uranium*(III)
$C_{12}H_{36}B_3O_3U$ M 498.8
Dark brown triclinic cryst. *fac*-Octahedral struct.

1,2-Bis(dimethylphosphino)ethane complex: [*1,2-Ethanediylbis(dimethylphosphine)*-P,P′] *tris(tetrahydroborato*-H,H′)*uranium*(III)
$C_{12}H_{44}B_3P_2U$ M 520.8
Olive cryst. Sol. Et_2O. Borohydrides are bidentate.

Bis(diphenyl-2-pyridinylphosphine) complex: Bis(diphenyl-2-pyridinylphosphine)tris(tetrahydroborato-H,H′,H″) *uranium*(III)
$C_{34}H_{40}B_3N_2P_2U$ M 809.1
Purple cryst. Sol. C_6H_6.

Schlesinger, M.J. *et al, J. Am. Chem. Soc.*, 1953, **75**, 219 (*synth*)
Volkov, V., *Radiokhimiya*, 1976, **8**, 512 (*synth*)
Moody, D.C. *et al, J. Inorg. Nucl. Chem.*, 1979, **41**, 533 (*synth*)
Ghiasseg, N. *et al, J. Inorg. Nucl. Chem.*, 1981, **43**, 2909 (*synth, ir*)
Wassermann, H.J. *et al, J. Chem. Soc., Chem. Commun.*, 1984, 532, 533 (*derivs, cryst struct, ir*)
Fazakerley, G.V. *et al, Polyhedron*, 1984, **3**, 457 (*synth, pmr, B-11 nmr*)
Männig, D. *et al, Z. Anorg. Allg. Chem.*, 1986, **543**, 66 (*synth, deriv, cryst struct, pmr, ir*)

$B_3H_{12}Y$ IC-001061

Yttrium(*III*) borohydride

Tris(tetrahydroborato(1−)-H,H′]yttrium(III), *10CI*

[72033-96-6]

$Y(BH_4)_3$

M 133.4

Bis-THF complex: Transparent colourless air- and moisture-sensitive cryst. Sol. THF. Subl. 90° *in vacuo*. Two kinds of Y, octahedral coord. by 4THF, $2BH_4$, or tetrahedral, coord. by $4BH_4$.

Tris-THF complex: [65415-37-4].
Air-sensitive colourless cryst. Sol. THF.

Rossmanith, K., *Monatsh. Chem.*, 1961, **92**, 768 (*synth*)
Bernstein, E.R. *et al, Chem. Phys.*, 1975, **10**, 215 (*synth*)
Segal, B.G. *et al, Inorg. Chem.*, 1978, **17**, 844 (*cryst struct*)
Lobkovskii, E.B. *et al, Zh. Strukt. Khim.*, 1982, **23**, 111; *J. Struct. Chem. USSR (Engl. Transl.)*, **23**, 582 (*cryst struct*)
Mancini, M. *et al, Inorg. Chem.*, 1984, **23**, 1072 (*pmr*)

$B_3H_{12}Yb$ IC-001062

Ytterbium(*III*) borohydride

Tris[tetrahydroborato(1−)-H,H′]ytterbium(III), *10CI*

[71722-79-7]

$Yb(BH_4)_3$

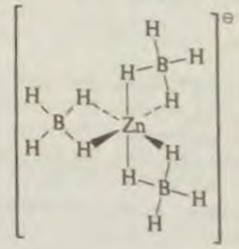
M 217.5
Obtd. as THF complex.

Tris-THF complex: [71896-59-8]. *Tris(tetrahydroborato) tris(tetrahydrofuran)ytterbium*(III)
$C_{12}H_{36}B_3O_3Yb$ M 433.8
Grey-white solid. Sol. THF.

Zange, E., *Chem. Ber.*, 1960, **93**, 652 (*synth*)
Mirsaidov, U. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1979, **15**, 1585; *Inorg. Materials (Engl. Transl.)*, 1980, **15**, 1248.
Mirsaidov, U. *et al, Zh. Neorg. Khim.*, 1983, **28**, 340; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 189 (*synth*)

$B_3H_{12}Zn^{\ominus}$ IC-001063

Tris[tetrahydroborato(1−)-*H,H′*]zincate(1−)



M 109.9 (ion)
Most solid solvated salts can be kept without dec. <0° in an inert atm. Salts obt. from zinc dihalides and MBH_4 (M = Li or Na) in ethereal solns.

▷ Salts hydrolyse violently with ignition.

Li salt, Et_2O complex: [35396-87-3].
Solid.

Na salt, Et_2O complex: [35396-88-4].
Solid.

Na salt, bis-THF complex: Solid. Mp −85°. Dec. into components at −25°.

K salt: [69916-45-6].
Solid.

Rb salt, bis(diglyme) complex: [56083-94-4].
Solid. Mp −18°. Dec. into components at 37°.

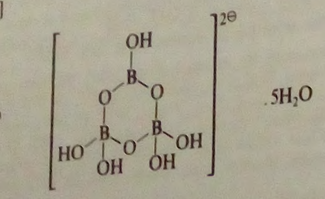
Cs salt, Et_2O complex: [70045-78-2].
Solid. Insol. Et_2O. Dec. at 125°.

Nöth, H. *et al, Z. Anorg. Allg. Chem.*, 1971, **386**, 73 (*synth, B-11 nmr, ir*)
Mikhaeva, V.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 225 (*synth, thermal anal, ir*)
Mal'tseva, N.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1989, **34**, 806 (*synth, ir*)

$B_3H_{15}MgO_{13}$ IC-001064

Magnesium triborate pentahydrate

[1318-70-3]



M 279.8

Can also be formulated $2MgO.3B_2O_3.15H_2O$.

Mineral-form [12260-26-3]

Inderite

Occurs in large quantities in Open Pit at Boron and other borate mining areas in California. Also found in USSR and Turkey. Colourless cryst., aggregates white to pink. This 2:3:15 compd. dec. thermally to give 2:3:1, 1:2:9, and 1:1:3 compds.

Schaller, W.T. *et al*, *Am. Mineral.*, 1960, **45**, 732 (*synth*)
Rumanova, I.M. *et al*, *Kristallografiya*, 1963, **8**, 517 (*cryst struct*)
Abdullaev, G.K. *et al*, *CA*, 1972, **77**, 96408 (*thermal anal*)
Corazza, E., *Acta Crystallogr., Sect. B*, 1976, **32**, 1329 (*cryst struct*)
Gode, H. *et al*, *CA*, 1976, **84**, 159004; 1981, **95**, 214226 (*synth, ir*)
Turner, G.L. *et al*, *J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)

$B_3K_3O_6$ IC-001065

Potassium triborate ($K_3B_3O_6$)

Potassium metaborate. Boric acid (HBO_2) potassium salt, 8CI

[13709-94-9]

$K_3B_3O_6$

M 245.7

Struct. comprises $K^{\oplus}$ cations and cyclic $B_3O_6^{3\ominus}$ anions. Synth. by melting together KO_2 and B_2O_3 in molar ratio (2:1). Used in photographic bleaching solns. Colourless hexagonal cryst. Sol. H_2O. Mp 947°. ΔH_f° −996 kJ mol^{-1}; ΔG_f° −937 kJ mol^{-1}; S° 80 J K^{-1} mol^{-1}.

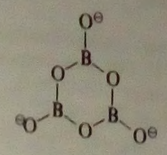
'Monomer': Potassium metaborate (KBO_2)
BKO_2 M 81.9

Zachariasen, W.H., *J. Chem. Phys.*, 1937, **5**, 919 (*cryst struct*)
Hart, P.B. *et al*, *J. Inorg. Nucl. Chem.*, 1962, **24**, 1047 (*ir*)
Tolédano, P., *Rev. Chim. Minér.*, 1964, **1**, 353 (*synth*)
Epperlein, B.W. *et al*, *Z. Naturforsch., A*, 1975, **30**, 955 (*B-10 nmr, B-11 nmr*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 238 (*thermochem data*)
Skvortsov, V.G., *Zh. Neorg. Khim.*, 1985, **30**, 2341 (*uv*)

$B_3O_6^{3\ominus}$ IC-001066

Triborate(3−), 9CI, 8CI

[20265-74-1]



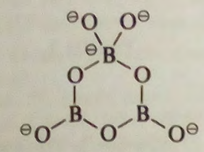
M 128.4 (ion)

Tri-Na salt: [19415-76-0]. *α-Trisodium triborate. Sodium triborate ($Na_3B_3O_6$)*
$B_3Na_3O_6$ M 197.3
Colourless cryst. Sol. H_2O.

Tri-K salt: see *Potassium triborate ($K_3B_3O_6$)*, IC-001065
Marezio, M. *et al*, *Acta Crystallogr.*, 1963, **16**, 594 (*cryst struct*)
Kriz, H.M. *et al*, *J. Magn. Reson.*, 1971, **4**, 76 (*rev, B-11 nmr*)
Bril, T.W., *Philips Res. Rep., Suppl.*, 1976, 114 (*ir, raman*)
Farmer, J.B., *Adv. Inorg. Chem. Radiochem.*, 1982, **25**, 187 (*rev, bibl*)

$B_3O_7^{5\ominus}$ IC-001067

Triborate(5−)



M 144.4 (ion)

Suggested struct. from X-ray powder data.

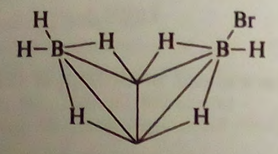
Ca, Al salt: ***Johachidolite***
AlB_3CaO_7 M 211.4
Mineral from Korea. White cryst.

Moore, P.B. *et al*, *Nature (London)*, 1972, **240**, 63 (*synth*)
Aristarain, L.F. *et al*, *Am. Mineral.*, 1977, **62**, 327 (*powder struct*)

B_4BrH_9 IC-001068

2-Bromotetraborane(10)

[36730-91-3]



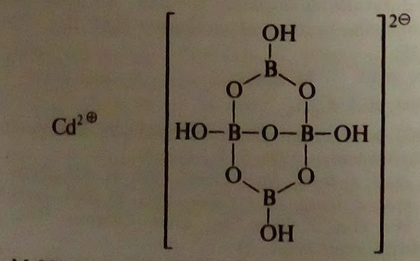
M 132.2

arachno-. Synth. from $[Bu_4N][B_3H_7Br]$ with BBr_3 in CH_2Cl_2 at −78°. Purif. by low temp. fractionation. Sol. CH_2Cl_2.

Shore, S.G. *et al*, *Inorg. Chem.*, 1982, **21**, 1952 (*synth, B-11 nmr, pmr, ir*)

$B_4CdH_{10}O_{12}$ IC-001069

Cadmium tetraborate pentahydrate



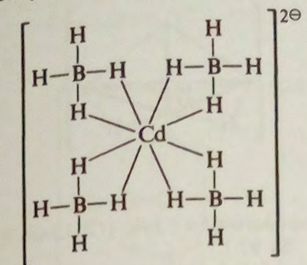
M 357.7

Also formulated $CdO.2B_2O_3.5H_2O$. White solid. Spar. sol. dil. HOAc. Loses one H_2O at 100°, a further three between 100-150° and the last H_2O at >300°.

Kesans, A. *et al*, *CA*, 1955, **50**, 14426 (*synth, thermal anal*)
Bokii, G.B. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1966, **7**, 860 (*cryst struct*)

$B_4CdH_{10}^{2\ominus}$ IC-001070

Tetrakis[tetrahydroborato(1−)-*H,H'*]cadmate(2−), 9CI



M 171.7 (ion)

Di-Li salt: [37080-48-1]. *Cadmium lithium borohydride*
$B_4CdH_{16}Li_2$ M 185.6
Oil.

Nöth, H. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **389**, 225 (*synth*)

B_4CeRh_4 IC-001071

Cerium rhodium boride ($CeRh_4B_4$), 10CI

[79986-46-2]

$CeRh_4B_4$

M 594.9

Obtd. in solid solns. with MRh_4B_4 (M = Lu etc.). Not isol. as pure substance, except by high pressure synth. Superconductor at v. low temps. (< 0.29K). Low T_c ascribed to valence fluctuation of Ce moments.

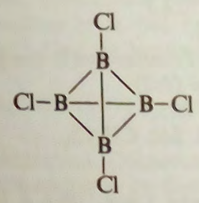
Delong, L.E. *et al*, *Ternary Supercond., Proc. Int. Conf., 1980*, (Shenoy, G.K. *et al*, Eds.), Elsevier, 1981, 193.
Shimotomai, M. *et al*, *J. Less-Common Met.*, 1987, **135**, 101 (*synth, magnetism*)
Ooyama, T. *et al*, *Physica B+C (Amsterdam)*, 1987, **148**, 133 (*synth*)

B_4Cl_4 IC-001072

Tetrachlorotetraborane(4), 11CI

Boron chloride (B_4Cl_4), 10CI, 9CI, 8CI. Tetraboron tetrachloride

[17156-85-3]



M 185.0

Tetrahedral molecule. Yellow cryst. easily hydrol. but mod. thermally stable. Sol. BCl_3. Mp 95°.

Atoji, M. *et al*, *Acta Crystallogr.*, 1953, **6**, 547 (*cryst struct*)
Massey, A.G. *et al*, *J. Chem. Soc.*, 1965, 6180 (*uv*)
Massey, A.G. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 365 (*ms*)
Kane, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 378 (*synth*)
Lloyd, D.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 627 (*pe*)
Brown, F.R. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 125 (*ir, raman*)
Davan, T. *et al*, *Inorg. Chem.*, 1979, **18**, 3194 (*synth, B-11 nmr, stability*)

B_4DyRh_4 IC-001073

Dysprosium rhodium boride ($DyRh_4B_4$), 10CI

[62974-26-9]

$DyRh_4B_4$

M 617.3

Forms solid solns. with other ternary metal borides. Ferromagnetic (T_c 12.03K).

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*struct*)
MacKay, H.B. *et al*, *J. Low Temp. Phys.*, 1980, **41**, 639 (*magnetic struct.*)
Stewart, A.M., *Phys. Rev. B*, 1985, **32**, 3331.
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)

B_4ErRh_4 IC-001074

Erbium rhodium boride ($ErRh_4B_4$), 10CI

[62974-27-0]

$ErRh_4B_4$

M 622.1

Antiferromagnetic superconductor. Tetragonal phase is superconductor at low temp. (T_c ~8.2K). Superconductivity destroyed by transition to ferromagnetic state at 0.9K.

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*synth, magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*struct*)
Woolf, L.D. *et al*, *J. Low Temp. Phys.*, 1979, **35**, 651 (*conductivity*)
Watanabe, Y. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 1644 (*synth, cryst struct*)
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)
Kakani, S.L. *et al*, *Phys. Status Solidi A*, 1987, **99**, 15 (*rev*)

B_4EuRh_4 IC-001075

Europium rhodium boride ($EuRh_4B_4$), 10CI

[66506-04-5]

$EuRh_4B_4$

M 606.8

Pure phase not isol.: can be stabilised by incorporation of 15% Ru or as solid solns. with other ternary lanthanide borides. Ru-containing phase is superconducting below *ca.* 1.5-2.0K.

[114705-54-3]

Johnston, D.C., *Solid State Commun.*, 1977, **24**, 699.
Delong, L.E. *et al*, *Ternary Supercond., Proc. Int. Conf., 1980*, Shenoy, G.K. *et al*, Eds., Elsevier, 1981, 193.
Iwazaki, H. *et al*, *Physica B+C (Amsterdam)*, 1987, **148**, 121.

B_4GdRh_4 IC-001076

Gadolinium rhodium boride ($GdRh_4B_4$), 10CI

[62974-28-1]

$GdRh_4B_4$

M 612.1

Forms solid solns. with MRh_4B_4 (M = Y, Er, Lu). Ferromagnetic (T_c 5.6K).

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*magnetism*)

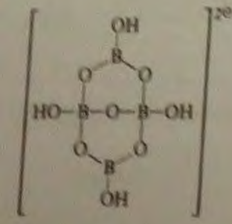
Vandenberg, J.M. *et al, Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*struct*)
Kuz'ma, Yu.B. *et al, J. Less-Common Met.*, 1979, **67**, 51 (*synth*)
Mackay, H.B. *et al, J. Low Temp. Phys.*, 1980, **41**, 639 (*magnetism*)
Adrian, H. *et al, Phys. Rev. B*, 1982, **26**, 2450 (*magnetism*)
Radcouky, H.B. *et al, Phys. Rev. B*, 1983, **27**, 4236 (*supercond*)
Lambert, S.E. *et al, Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)

$B_2H_4O_9^{2\ominus}$ IC-001077

Tetraborate(2−)

Tetrahydrogen tetraborate, 9CI. Borate (B_4O_9)$^{2\ominus}$, tetrahydrogen, 8CI

[12344-83-1]



M 191.2 (ion)

Di-Na salt, trihydrate: see *Disodium tetraborate pentahydrate, IC-001086*

Di-Na salt, octahydrate: see *Borax, IC-001088*

Di-K salt, dihydrate: see *Dipotassium tetraborate dihydrate, IC-001081*

Di-Cs salt:
$B_4Cs_2H_4O_9$ M 457.0
Colourless cryst. Sol. H_2O.

Mn(II) salt, heptahydrate: see *Manganese tetraborate heptahydrate, IC-001097*

Cd salt, trihydrate: see *Cadmium tetraborate pentahydrate, IC-001089*

Di-NH_4 salt, dihydrate: see *Diammonium tetraborate tetrahydrate, IC-001085*

[21772-81-6]

Marezio, M. *et al, Acta Crystallogr.*, 1963, **16**, 975 (*cryst struct*)
Spessard, J.E., *J. Inorg. Nucl. Chem.*, 1970, **32**, 2607 (*synth*)
Janda, R. *et al, Z. Naturforsch., B*, 1979, **34**, 585 (*ir, raman*)
Farmer, J., *Adv. Inorg. Chem. Radiochem.*, 1982, **25**, 187 (*rev, bibl*)
Salentine, C.G., *Inorg. Chem.*, 1983, **22**, 3920 (*B-11 nmr*)

$B_4H_4Li_2O_{10}$ IC-001078

Dilithium tetraborate trihydrate

$Li_2O.2B_2O_3.3H_2O$

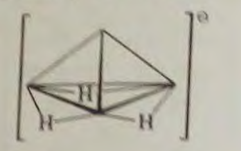
M 223.1

Evidence that this compd. is a tetra- rather than tri-hydrate is unconvincing. Colourless cryst. Mod. sol. H_2O.

Bouaziz, R., *Bull. Soc. Chim. Fr.*, 1962, 1451 (*thermal anal*)
Perry, G.S., *Chem. Ind. (London)*, 1964, 1025 (*struct*)
Benhassaine, A., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1516 (*synth*)

$B_4H_7^{\ominus}$ IC-001079

Heptahydrotetraborate(1−), 9CI, 8CI



M 50.2 (ion)

nido-.

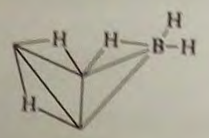
Diammine(dihydro)boron(1+) salt: [12513-01-8].
$B_5H_{15}N_2$ M 97.1
Colourless solid. Sol. liq. NH_3. Unstable at r.t.

Kodama, G., *J. Am. Chem. Soc.*, 1970, **92**, 3482 (*synth*)
Kodama, G. *et al, J. Am. Chem. Soc.*, 1972, **94**, 407 (*synth, B-11 nmr*)

B_4H_8 IC-001080

Tetraborane(8), 11CI, 10CI, 9CI, 8CI

[12007-71-5]



M 51.3

Unstable borane - stabilised as complexes.

CO complex: [12539-64-9]. *Tetraborane(8) carbonyl*
CH_8B_4O M 79.3
Colourless gas. Mp −113° - −110°. Mixt. of two stereoisomers, *exo-* and *endo-CO*.

NMe_3 complex: Tetraborane(8) compd. with Me_3N (1:1)
$C_3H_{17}B_4N$ M 110.4
Colourless cryst. Sol. ethers, CH_2Cl_2. Mp ~40°.

TMED complex: Tetraborane(8) complex with tetramethylethylenediamine (1:1)
$C_6H_{24}B_4N_2$ M 167.5
Sol. MeCN, DMSO.

PMe_3 complex: [71749-92-3]. *Tetraborane(8) complex with trimethylphosphine (1:1)*
$C_3H_{17}B_4P$ M 127.3
Sublimeable solid.

Bis-PMe_3 complex: Tetraborane(8) complex with trimethylphosphine (1:2)
$C_6H_{26}B_4P_2$ M 203.4
Sublimeable solid. Sol. CH_2Cl_2.

[59035-20-0]

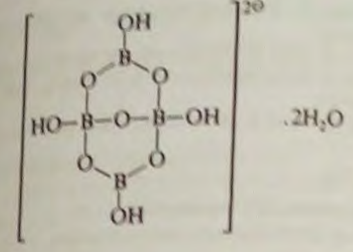
Spielman, J.R. *et al, Inorg. Chem.*, 1963, **2**, 1139 (*synth, ir, B-11 nmr*)
Miller, N.E. *et al, Inorg. Chem.*, 1964, **3**, 866 (*synth, ir, pmr, B-11 nmr*)
Hollins, R.E. *et al, Inorg. Chem.*, 1970, **9**, 877 (*ms*)
Onak, T.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2633 (*synth*)
Stampf, E.J. *et al, Inorg. Chem.*, 1975, **14**, 2446 (*pmr, B-11 nmr*)
Colquhoun, H.M., *J. Chem. Res. (S)*, 1978, 451 (*pmr, B-11 nmr*)
Dodds, A.R. *et al, Inorg. Chem.*, 1979, **18**, 1465 (*synth, ms, pmr, B-11 nmr*)
Kodama, G., *Inorg. Chem.*, 1979, **18**, 3302 (*synth, ms, pmr, B-11 nmr, P-31 nmr*)
Kameda, M. *et al, Inorg. Chem.*, 1984, **23**, 3205 (*synth, ms, pmr, B-11 nmr, P-31 nmr*)
McKee, M.L., *J. Am. Chem. Soc.*, 1990, **112**, 6753 (*theory*)

$B_2H_6K_2O_{11}$ IC-001081

Dipotassium tetraborate dihydrate, 9CI

Dipotassium tetraborate tetrahydrate. Boron potassium oxide ($B_4K_2O_7$) tetrahydrate,11CI, 10CI, 9CI

[12045-78-2]



M 305.4

Used as borax substitute when greater aq. solubility is required or when absence of $Na^{\oplus}$ necessary. Colourless orthorhombic cryst. Sol. H_2O. Loses two H_2O between 112-195°, a third at 195-200° and the last between 240-420°.

Marezio, M. *et al, Acta Crystallogr.*, 1963, **16**, 975 (*cryst struct*)
Weir, C.E., *J. Res. Natl. Bur. Stand., Sect. A*, 1966, **70**, 153 (*ir*)
Stavrs, E. *et al, CA*, 1968, **69**, 83095 (*thermal anal*)
Toledano, P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 412 (*synth*)
Krogh-Moe, J. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 3089 (*cryst struct*)
Anferov, V.P. *et al, CA*, 1985, **103**, 226096 (*nmr, nqr*)

$B_2H_6Na_2O_{11}$ IC-001082

Disodium tetraborate tetrahydrate

[12045-87-3]

$Na_2[B_4O_5(OH)_2].3H_2O$

M 273.2

Struct. contains parallel infinite chains of $[B_4O_5(OH)_2]_n^{2n\ominus}$ anions - two B atoms are 4-coordinate and two are 3-coordinate in the B_4 structural unit. Also formulated as $Na_2O.2B_2O_3.4H_2O$. Manuf. directly from the mineral. Used in prodn. of sodium perborate, a bleaching agent in washing powders. Used in manuf. of glass fibre, cellular insulation, borosilicate glasses and enamels. Colourless monoclinic cryst. Sol. hot H_2O. ΔH_f° −4481.9 kJ mol^{-1}. Dec. on heating: $-2H_2O$ at 60°, $-4H_2O$ at 320°.

Mineral-form [12447-37-9]
Kernite, 9CI
Occurs in e.g. Argentina. Colourless transparent cryst., tarnishes to white owing to surface formation of tincalconite.

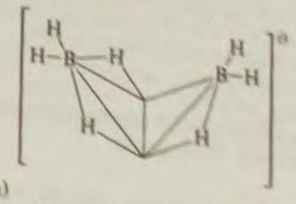
[12267-20-0]

Weir, C.E., *J. Res. Natl. Bur. Stand., Sect. A*, 1966, **70**, 153; *CA*, 1966, **65**, 6519 (*ir*)
Nies, N.P. *et al, J. Chem. Eng. Data*, 1967, **12**, 303 (*synth*)
Cooper, W.F. *et al, Am. Mineral.*, 1973, **58**, 21 (*cryst struct*)
Hurlbut, C.S. *et al, Am. Mineral.*, 1973, **58**, 308 (*cryst struct, thermal anal*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1980, V/A, 370 (*rev, bibl*)
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)

$B_4H_9^{\ominus}$ IC-001083

Nonahydrotetraborate(1−), 10CI

[12429-85-5]



M 52.3 (ion)

arachno-anion. Intermed. for synth. of tetraborane(10) derivs. and of pentaborane(11).

K salt:
B_4H_9K M 91.4
Colourless cryst. stable at −78°. Sol. ethers.

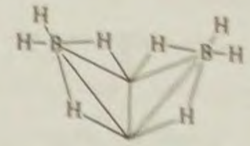
Tetrabutylammonium salt: Colourless cryst.

Johnson, H. *et al, J. Am. Chem. Soc.*, 1970, **92**, 7586 (*deriv*)
Reitz, R. *et al, Inorg. Chem.*, 1972, **11**, 1242 (*nmr*)
Remmel, R. *et al, J. Am. Chem. Soc.*, 1975, **97**, 5395 (*synth, nmr*)

B_4H_{10} IC-001084

Tetraborane(10), 10CI

[18283-93-7]



M 53.3

arachno-. Colourless gas or liq. Mp −120°. Bp 18°.

Leach, J.B. *et al, Inorg. Chem.*, 1970, **9**, 2170 (*nmr*)
Taft, M. *et al, Inorg. Chem.*, 1982, **21**, 1952 (*synth*)

$B_4H_{10}K_4O_{13}$ IC-001085

Potassium metaborate 1½ hydrate (or 1½ hydrate), 9CI

$K_2O.B_2O_3.2.5H_2O$

M 417.7

May be $K_2O.B_2O_3.2\frac{1}{2}H_2O$. Anion struct. is based on $[B_3O_4(OH)_4]^{2\ominus}$ units. Colourless cryst. Sol. H_2O. Loses H_2O at 164° and becomes anhydrous between 230-450°.

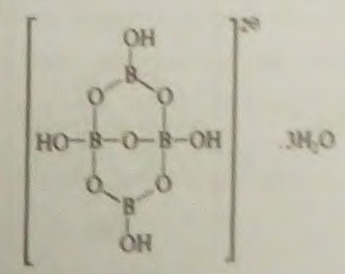
Toledano, P., *Rev. Chim. Minér.*, 1964, **1**, 353 (*synth, thermal anal*)
Jahr, K.F. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 1677 (*B-11 nmr*)
Toledano, P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 1141 (*synth*)
Kessler, G. *et al, Z. Anorg. Allg. Chem.*, 1969, **365**, 281 (*ir*)
Zviedre, I.I. *et al, CA*, 1972, **77**, 157462 (*cryst struct*)

$B_4H_{10}Na_2O_{12}$ IC-001086

Disodium tetraborate pentahydrate, 10CI, 9CI

Borax pentahydrate

[12228-99-8]



M 291.2
Commercially important feedstock for B-based fire retardants, detergents, herbicides, bleaches, agrochemicals, glasses. Colourless cryst. Sol. H_2O, EtOH, polyols. Up to three H_2O lost when heated to 140-150°, becomes anhydrous at ~400°.

Mineral-form [12045-88-4]
Tincalconite, 10Cl, 8Cl
Occurs as a hydration or dehydration product of other borate minerals. White powder.

[12228-94-3]
Coltheup, J.D. *et al, J. Chem. Phys.*, 1963, **38**, 1912 (*pmr, B-11 nmr*)
Weir, C.E., *J. Res. Natl. Bur. Stand., Sect. A*, 1966, **70**, 153; *CA*, 1966, **65**, 6519 (*ir*)
Nies, N.P. *et al, J. Chem. Eng. Data*, 1967, **12**, 303 (*synth*)
Jain, K.F. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 1677 (*pmr*)
Benhaoualine, A., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1516 (*synth, thermal anal*)
Giusseppetti, G. *et al, Am. Mineral.*, 1973, **58**, 523 (*cryst struct*)
Nies, N.P., *Mellor Compr. Treat. Inorg. Theor. Chem.*, Longman, London, 1980, **V/A**, 368 (*rev, bibl*)

$B_2H_{10}Hf$ IC-001087

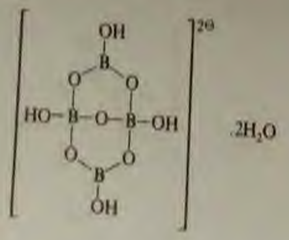
Hafnium(*IV*) borohydride
Tetrakis(tetrahydroborato(1−)-H,H′H″)hafnium, 11Cl
[55608-70-1]

M 237.8
Molecular with strict T_d symmetry. Synth. by reaction of $HfCl_4$ and $LiBH_4$ in Et_2O and purified by low temp. trap to trap distillation. Colourless, v. moisture sensitive solid. A form in which two H bridge to the Hf based on vibrational spectra is probably the same compd.

[25869-93-6, 37274-93-4]
James, B.D. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1974, **4**, 461 (*synth*)
Wozniak, W.T. *et al, Inorg. Chem.*, 1975, **14**, 576 (*ir, raman*)
Hitchcock, A.P. *et al, Inorg. Chem.*, 1982, **21**, 793 (*synth, pe*)
Broach, R.W. *et al, Inorg. Chem.*, 1983, **22**, 1081 (*nd*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1834.

$B_4H_{16}N_2O_{11}$ IC-001088

Diammonium tetraborate tetrahydrate
[10135-84-9]



M 263.3
Used as borate source when alkali metal ions are specifically not required. Used in manuf. of urea-formaldehyde foams, fire retardants and in electrochemistry. Colourless cryst; quite unstable at r.t., evolves NH_3. Sol. H_2O.

Toledano, P. *et al, Bull. Soc. Chim. Fr.*, 1966, 1933; 1969, 1462 (*synth*)
Janda, R. *et al, Z. Naturforsch., B*, 1979, **34**, 1078 (*B-11 nmr*)
Janda, R. *et al, Spectrochim. Acta, Part A*, 1980, **36**, 997 (*ir, raman*)
Janda, R. *et al, Z. Kristallogr.*, 1981, **154**, 1 (*cryst struct*)

$B_4H_{16}Np$ IC-001089

Neptunium(*IV*) borohydride
Tetrakis(tetrahydroborato)neptunium
[66615-98-3]

$Np(BH_4)_4$

M 296.4
12-Coordinate, monomeric. Most volatile Np(*IV*) compd. known. Dark green liq. Mp 14.2°. V. volatile, V.p. 10mm Hg at 25°. Isostructural with Plutonium(*IV*) borohydride, IC-001091 (not $U(BH_4)_4$) and similar to Zr, Hf analogues.
▷ Pyrophoric.

Banks, R.H. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1957; 1980, **102**, 620 (*synth, ir, cryst struct*)
Solar, J.P. *et al, Inorg. Chem.*, 1980, **19**, 2186 (*use*)

$B_4H_{16}Pa$ IC-001090

Protactinium(*IV*) borohydride
Tetrakis[tetrahydroborato(1−)]protactinium(IV)
[66614-96-8]

$Pa(BH_4)_4$

M 290.4
Red-orange air-sensitive solid. Subl. 55° *in vacuo*. Isostructural with $U(BH_4)_4$.

[77340-17-1]
Banks, R.H. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1957 (*synth*)
Banks, R.H. *et al, ACS Symp. Ser.*, 1980, **131**, 331 (*synth*)

$B_4H_{16}Pu$ IC-001091

Plutonium(*IV*) borohydride
Tetrakis[tetrahydroborato(1−)-H,H′,H″]plutonium(IV), *10Cl*
[66615-99-4]

$Pu(BH_4)_4$

M 298.4
12-Coordinate with tridentate BH_4. Monomeric. Blue-black volatile liq. Mp 15°. Isostructural with Np analogue, Neptunium(*IV*) borohydride, IC-001089. Thermally unstable.

Banks, R.H. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1957 (*synth, ir*)
Banks, R.H. *et al, ACS Symp. Ser.*, 1980, **131**, 331.
Solar, J.P. *et al, Inorg. Chem.*, 1980, **19**, 2186 (*use*)

$B_4H_{16}Th$ IC-001092

Thorium(*IV*) borohydride
Tetrakis[tetrahydroborato(1−)-H,H′]thorium(IV)
[12523-76-1]

$Th(BH_4)_4$

M 291.4

14-Coordinate, polymeric struct. with two terminal tridentate BH_4 and four bridging bidentate BH_4 groups. Air-sensitive white cryst. Mp 204° dec. Subl. 140° *in vacuo*. Isostructural with U analogue.

Hoekstra, H.R. *et al, J. Am. Chem. Soc.*, 1949, **71**, 2488 (*synth*)
Eisenmann, M. *et al, Z. Anorg. Allg. Chem.*, 1971, **386**, 87 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1163 (*synth*)
Banks, R.H. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1957 (*synth*)
Le Vanda, C. *et al, J. Am. Chem. Soc.*, 1980, **102**, 2129 (*use*)

$B_2H_{10}Ti^{\odot}$ IC-001093

Tetrakis(tetrahydroborato)titanate(*III*)(1−)
Tetrakis(tetrahydroborato(1−)-H,H′)bis[tetrahydroborato(1−)-H,H′]titanate(1−), 11Cl. Tetrakis(borohydrido) titanate(III)(1−)

$[Ti(BH_4)_4]^{\odot}$

M 107.2 (ion)
Detailed struct. is not known.
Tris[(1,2-dimethoxyethane)sodium] salt: [101307-98-6].
Synth. from $TiCl_4$ and $NaBH_4$ in dimethoxyethane.

Borisov, A.P. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1986, **31**, 47 (*synth, ir*)

$B_2H_{10}U$ IC-001094

Uranium borohydride
Tetrakis(tetrahydroborato)uranium, 10Cl
[18903-76-3]

$U(BH_4)_4$

M 297.3
Uranium is 14-coordinate. Exists in two cryst. forms. Yellow-green cryst. or emerald-green cryst. Sol. heptane, C_6H_6. Dissolves in ethers (Et_2O, THF) forming adducts. Air- and moisture-sensitive. Stable below 70°. Highly volatile.

Me_2O complex: [65150-32-5].
$C_3H_{12}B_4OU$ M 343.4
Air- and moisture-sensitive cryst. Sol. Me_2O. Mp 93°. Subl. 20° *in vacuo*.
▷ Inflames in contact with water.

Et_2O complex: [65150-21-2].
$C_4H_{20}B_4OU$ M 381.6
Air- and moisture-sensitive green cryst. Sol. Et_2O. Mp 66°. Subl. 20° *in vacuo*.
▷ Inflames in contact with water, sometimes explosively.

Bis-THF complex: [65167-99-9].
$C_8H_{28}B_4O_2U$ M 441.6
Air- and moisture-sensitive pale-green cryst. Sol. THF. Mp 122° dec. Subl. 50-60° *in vacuo*.
▷ Inflames in contact with water.

Dipropyl ether complex: [65150-34-7].
$C_6H_{30}B_4OU$ M 367.1
Air- and moisture-sensitive light-green solid. Sol. dipropyl ether. Mp 62-63°. Subl.$_{0.0001}$ 30-40°. Dimeric.

1,2-Dimethoxyethane complex:
$C_4H_{28}B_4O_2U$ M 387.5
Green cryst. Sol. toluene.

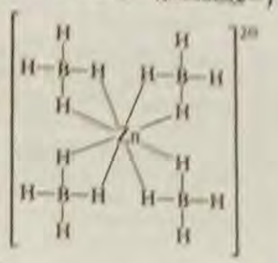
Bis-HMPA complex:
$C_{20}H_{52}B_4N_6O_2P_2U$ M 637.6
Pale-green microcryst. Sol. toluene.

Bis-Ph_3PO complex:
$C_{56}H_{48}B_4O_2P_2U$ M 853.9
Pale-green microcryst. Sol. CH_2Cl_2.

Schlesinger, H.I. *et al, J. Am. Chem. Soc.*, 1953, **75**, 219 (*synth*)
Bernstein, E.R. *et al, Inorg. Chem.*, 1972, **11**, 3009 (*cryst struct*)
Bernstein, E.R. *et al, J. Am. Chem. Soc.*, 1972, **94**, 2552 (*cryst struct*)
Bernstein, E.R. *et al, J. Chem. Phys.*, 1973, **59**, 2105 (*synth, ms-ais*)
Rietz, R.R. *et al, Inorg. Chem.*, 1978, **17**, 653, 658, 661 (*cryst struct, deriv*)
Paine, R.J. *et al, Spectrochim. Acta, Part A*, 1979, **35**, 213 (*ir*)
Charpin, P. *et al, Acta Crystallogr., Sect. C*, 1987, **43**, 1255, 1463, 1630 (*synth, cryst struct*)
Baudry, D. *et al, J. Organomet. Chem.*, 1988, **349**, 123 (*synth, pmr, ir*)

$B_4H_{16}Zn^{2\odot}$ IC-001095

Tetrakis[tetrahydroborato(1−)]zincate(2−)



M 124.7 (ion)
Di-Li salt, tris-Et_2O complex: [35397-81-0]. Cryst.
Ca salt, tris-Et_2O complex: [69916-48-9]. Solid. Dec. at 120°.
Ca salt, tris(diglyme) complex: [69916-50-3]. Solid. Dec. at 140°.
Ba salt, tris-Et_2O complex: [69916-52-5]. Dec. at 120°.

Nöth, H. *et al, Z. Anorg. Allg. Chem.*, 1971, **386**, 73 (*synth, B-11 nmr, ir*)
Mikhaeva, V.I. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 225 (*synth, thermal anal, ir*)

$B_4H_{16}Zr$ IC-001096

Tetrakis[tetrahydroborato(1−)-*H,H′,H″*]zirconium(*IV*), 11Cl
Zirconium(IV) *borohydride. Tetrakis(borohydrido) zirconium*(IV). *Zirconium tetrakis(tetrahydroborate)*
[12370-59-1]

$Zr(BH_4)_4$

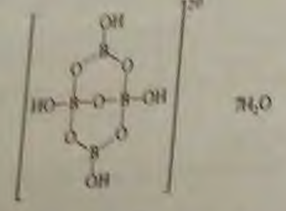
M 150.5
Tetrahedral molecule. Synth. from a slurry of $ZrBr_4$ and $LiBH_4$ in ether or by milling solid $ZrCl_4$ and $NaBH_4$. Used in ethylene polym. catalysts and to form ZrB_2 coatings on nuclear fuel elements. Air, moisture and light-sensitive colourless low-melting solid. Mp 28.7°. Bp 123° (extrap.). Thermal dec. yields ZrB_2.

Bird, P.M. *et al, J. Chem. Soc., Chem. Commun.*, 1967, 403 (*cryst struct*)
Plato, V. *et al, Inorg. Chem.*, 1971, **10**, 590 (*ed*)
Marks, T.J. *et al, Inorg. Chem.*, 1972, **11**, 2540 (*ir, raman, esr*)
James, B.D. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1974, **4**, 461 (*synth*)
Smith, B.E. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 710 (*ir, raman*)
Sayer, B.G. *et al, Inorg. Chem.*, 1981, **20**, 3748 (*pmr, B-11 nmr, Zr-91 nmr*)
Fr. Pat., 2 567 542, (1986); *CA*, **105**, 104470f (*use*)
Nesterov, G.A. *et al, J. Mol. Catal.*, 1986, **36**, 253 (*use*)

$B_2H_{10}MnO_{14}$ IC-001097

Manganese tetraborate heptahydrate, 10CI, 9CI

[55280-02-5]



M 372.3

Also formulated as $MnO.2B_2O_3.6H_2O$. Commercially available. Pinking ink drier. Solid. Sol. H_2O. Six H_2O lost between 50-70°, from 70-100° one more H_2O is lost but final $2H_2O$ are not lost until > 350°.

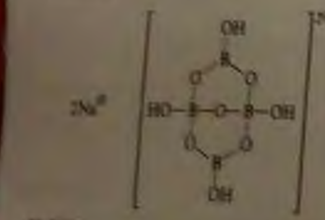
Berzina, I. *et al*, *CA*, 1975, **82**, 7911 (*cryst struct*)
Gioth, I. *et al*, *CA*, 1979, **90**, 130736 (*thermal anal*)
Nies, N.P., *Mellor Compr. Treat. Inorg. Theor. Chem.*, Longman, London, 1980, V/A, 633 (*comb, rev, bibl*)

$B_4H_{20}Na_2O_{17}$ IC-001098

Borax, 11Cl, 10Cl, 9Cl, 8Cl

Tincal. Disodium tetraborate decahydrate. Borax decahydrate. Sodium borate

[1303-96-4]



M 381.3

The most important commercial borate. Also formulated as $Na_2O.2B_2O_3.10H_2O$. Feedstock for borate-based detergents, agrochemicals, fire retardants, photographic chemicals, textile finishes and glasses. Colourless monoclinic cryst. Sol. H_2O (2 g per 100 cm^3 at 0°, 170 g per 100 cm^3 at 100°) MeOH, polyols; spar. sol. Me_2CO, EtOAc, EtOH. Stable in aq. soln. up to 61° then dehydrates to Disodium tetraborate pentahydrate. IC-001086 - complex dehydration reactions depend somewhat on sample's history.

▷ VZ2275000

Mineral-form

Borax

Occurs as a deposit from hot springs and in evaporated saline lake and playa deposits. Widespread occurrence in California. Also found in Mexico, Argentina, Tibet, Iran, USSR and Turkey. Colourless or white to greyish, greenish or bluish cryst.

[1344-80-7, 12322-85-8, 12447-40-4, 61028-24-8, 71377-02-1]

Thenius, O., *Monatsh. Chem.*, 1950, **81**, 301 (*raman*)
Nies, N.P. *et al*, *J. Chem. Eng. Data*, 1967, **12**, 303 (*cryst*)
Thomas, G. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1972, **69**, 1154 (*thermal anal*)
Levy, H.A. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3502 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 80 (*manuf, uses, tox*)

Kochergin, V.P. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1641 (*prep, B-11 nmr*)
Nies, N.P., *Mellor Compr. Treat. Inorg. Theor. Chem.*, Longman, London, 1980, V/A, 356 (*rev, bibl*)
Janda, R. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 997 (*ir, raman*)
Turner, G.L. *et al*, *J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3155C (*haz*)

B_4HoRh_4 IC-001099

Holmium rhodium boride ($HoRh_4B_4$), 10CI

[62974-29-2]

$HoRh_4B_4$

M 619.7

Has $CeCo_4B_4$ struct. Forms range of solid solns. with other tertiary lanthanide borides. Superconductor. Antiferromagnetic (T_c ~6.6K).

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*struct*)
Ott, H.R. *et al*, *J. Low Temp. Phys.*, 1980, **39**, 383; 1983, **51**, 505 (*magnetism, contd*)
Kohara, T. *et al*, *Phys. Lett. A*, 1983, **96**, 425 (*B-11 nmr*)
Kohori, Y. *et al*, *J. Phys. Soc. Jpn.*, 1984, **53**, 780 (*nmr*)
Iwasaki, H. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 326 (*magnetism*)
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)
Adrian, H. *et al*, *Physica B+C (Amsterdam)*, 1987, **148**, 76 (*rel struct*)

$B_4K_2O_7$ IC-001100

Potassium tetraborate

Boric acid ($H_2B_4O_7$) dipotassium salt, 9Cl, 8Cl. Boron potassium oxide ($B_4K_2O_7$), 11Cl, 10Cl. Potassium biborate. Potassium borate. Dipotassium borate ($B_4O_7^{2\ominus}$)

[1332-77-0]

$K_2B_4O_7$

M 233.4

Synth. by melting together KO_2 and B_2O_3 in appropriate molar ratio. Used in detergents, photographic developing solns. and fire extinguishers. Colourless triclinic cryst., hygroscopic. Mp 815°. ΔH_f° −3334.2 kJ mol^{-1}; ΔG_f° −3136.8 kJ mol^{-1}; S° 208 J K^{-1} mol^{-1}.

Tetrahydrate: see *Dipotassium tetraborate dihydrate, IC-001084*

Miller, F.A. *et al*, *Anal. Chem.*, 1952, **24**, 1253 (*ir*)
Krogh-Moe, J., *Acta Crystallogr.*, 1961, **14**, 68 (*cryst struct*)
Toledano, P., *Rev. Chim. Miner.*, 1964, **1**, 353 (*synth*)
Epperlein, B.W. *et al*, *Z. Naturforsch., A*, 1975, **30**, 955 (*B-10 nmr, B-11 nmr*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 289 (*thermochem data*)
Skvortsov, V.G., *Zh. Neorg. Khim.*, 1985, **30**, 2341 (*sel*)

B_4LaRh_4 IC-001101

Lanthanum rhodium boride ($LaRh_4B_4$), 10CI

[80891-54-9]

$LaRh_4B_4$

M 593.7

Not isol. as pure phase, only in mixed $La_xLu(Rh_{0.85}Ru_{0.15})_4B_4$

Johnston, D.C., *Physica B+C (Amsterdam)*, 1981, **108**, 755.

$B_4Li_2O_7$ IC-001102

Lithium tetraborate

Boric acid, dilithium salt, 8CI

[12007-60-2]

$Li_2B_4O_7$

M 169.1

Prepared by thermal treatment of a 2:1 B_2O_3:Li_2O molar ratio. Commercially available. Spectroscopic fluxing agent; component of γ-ray thermoluminescent dosimeters. White tetragonal cryst. Mod. sol. H_2O (2.9 g per 100 cm^3 at 20°; 5.5 g per 100 cm^3 at 100°). Mp 917°. ΔH_f° −3362 kJ mol^{-1}; ΔG_f° −3170 kJ mol^{-1}; S° 156 J K^{-1} mol^{-1}.

▷ Irritant.

Gmelin Handbook Inorg. Chem., Syst. No 20, 1960, 491 (*rev, bibl*)
Krogh-Moe, J., *Acta Crystallogr.*, 1962, **15**, 190 (*cryst struct*)
Weir, C.E. *et al*, *J. Res. Natl. Bur. Stand., Sect. A*, 1964, **68**, 465 (*ir*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 292 (*thermochem data*)

B_4LuRh_4 IC-001103

Lutetium rhodium boride ($LuRh_4B_4$), 11CI

[62974-30-5]

$LuRh_4B_4$

M 629.8

Forms solid solns. with Ru analogue. Tetragonal phase is superconductor (T_c ~11.6K). Also exists as orthorhombic form.

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*cryst struct*)
Woolf, L.D. *et al*, *J. Low Temp. Phys.*, 1979, **35**, 651 (*props*)
Ott, H.R. *et al*, *Physica B+C (Amsterdam)*, 1981, **108**, 751 (*magnetism*)
Yvon, K. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 247 (*cryst struct*)
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)
Lee, W.H. *et al*, *J. Low Temp. Phys.*, 1987, **68**, 147 (*props*)
King, R.B., *J. Solid State Chem.*, 1987, **71**, 233 (*struct*)
Iwasaki, H. *et al*, *Physica B+C (Amsterdam)*, 1987, **148**, 121.

B_2MnO_7 IC-001104

Manganese tetraborate

Manganese(II) borate (MnB_4O_7), 11Cl

[12228-91-0]

MnB_4O_7

M 210.1

Orthorhombic. The B_4O_7 group consists of two tetrahedral BO_4 groups with a common O atom, each tetrahedron sharing two other O atoms with two BO_3 groups. $Mn^{2\oplus}$ occupies distorted tetrahedron of O atoms. Obt. by metathesis of aq. molar solns. of $MnSO_4$ and borax and washing the precipitate and drying at 500° for 4 h. Cryst. Mp 940°. ΔH_f° −75.3 kJ mol^{-1} (est.).

Nonahydrate: Synth. from $MnCl_2.4H_2O$ and $Na_2B_4O_7.10H_2O$ in H_2O. Light pink cryst. Structural composition is $Mn[B_4O_5(OH)_4].7H_2O$. Some studies have been done on a commercial product $MnB_4O_7.8H_2O$.

Mazzetti, C. *et al*, *Gazz. Chim. Ital.*, 1926, **56**, 19 (*mp*)
Khanikar, M.H. *et al*, *J. Indian Chem. Soc.*, 1963, **40**, 9 (*synth*)
Abrahams, S.C. *et al*, *J. Chem. Phys.*, 1974, **60**, 1899 (*synth, cryst struct, magnetism*)
Slough, W. *et al*, *CA*, 1975, **82**, 35533 (*thermochem data*)
Berzina, I. *et al*, *Struct. Rep. A*, 1975, **41**, 288 (*hydrate, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, C7, 63 (*prep, bibl*)

$B_4Na_2O_7$ IC-001105

Disodium tetraborate, 11Cl, 10Cl, 9Cl, 8Cl

Borax ($B_4Na_2O_7$), 10Cl. Boron sodium oxide ($B_4Na_2O_7$), 10Cl. Boric acid, disodium salt, 8Cl. Anhydrous borax. Borax, fused

[1330-43-4]

$Na_2O.2B_2O_3$

M 201.2

Known in three forms, α- and metastable β- and γ-forms. Contains $[B_8O_{14}]^{4\ominus}$ anions consisting of linked B_3O_3 and B_2O_6 groups. Feedstock for glass, glazes, fertilisers and welding or brazing fluxes. Colourless solid. Sol. H_2O (1.1 g per 100 cm^3 at 0°, 8.8 g per 100 cm^3 at 40°), MeOH, ethylene glycol. Mp 743° (α-form), Mp 720° (β-form), Mp 663° (γ-form). Bp 1575°. ΔH_f° −3259 kJ mol^{-1}; ΔG_f° −3082 kJ mol^{-1}; S° 189.5 J K^{-1} mol^{-1}.

▷ Irritant.

Monohydrate: [12447-36-8].
$B_4H_2Na_2O_8$ M 219.2
Colourless cryst. Sol. H_2O → $Na_2B_4O_7.5H_2O$. Correctly formulated as $Na_2B_4O_6(OH)_2$.

*Dihydrate: **Metakernite***
$B_4H_4Na_2O_9$ M 237.2
Mineral or prepd. by thermal dec. of $Na_2B_4O_7.10H_2O$ or $Na_2B_4O_7.4H_2O$ either under vacuum or over P_2O_5. Amorphous powder. Correctly formulated as $Na_2B_4O_5(OH)_4$.

Tetrahydrate: see *Disodium tetraborate tetrahydrate, IC-001082*

Pentahydrate: see *Disodium tetraborate pentahydrate, IC-001086*

Decahydrate: see *Borax, IC-001098*

Onak, T.P. *et al*, *J. Phys. Chem.*, 1959, **63**, 1533 (*B-11 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 266; 1966, **3**, 1271 (*rev, bibl*)
Thomas, G. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 4202 (*synth, dihydrate*)
Krogh-Moe, J., *Acta Crystallogr., Sect. B*, 1974, **30**, 578 (*cryst struct*)
Bertoluzza, A. *et al*, *CA*, 1974, **81**, 81583 (*ir, raman*)
Epperlein, B.W. *et al*, *Z. Naturforsch., A*, 1975, **30**, 955 (*B-10, B-11, D nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 90 (*manuf, uses*)
Nies, N.P., *Mellor Compr. Treat. Inorg. Theor. Chem.*, Longman, London, 1980, V/A, 383 (*rev, bibl*)
Fedulov, S.A. *et al*, *Inorg. Materials (Engl. Transl.)*, 1983, **19**, 445 (*thermal anal*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 296 (*thermodyn*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3155B (*haz*)

B_4NdRh_4 IC-001106

Neodymium rhodium boride ($NdRh_4B_4$), 10Cl

[62974-31-6]

$NdRh_4B_4$

M 599.1

Tetragonal phase is superconductor (T_c ~5.3K). Antiferromagnetic transitions occur at ~1.5 and ~1.0K (sat. μ_{sat} = 3.4μ_B).

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*synth*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*struct*)
Johnston, D.C., *Physica B+C (Amsterdam)*, 1981, **108**, 755.
Maple, M.B., *Ternary Supercond., Proc. Int. Conf., 1980*, Shenay, G.K. *et al*, Eds., Elsevier, 1981, 131 (*rev*)
Majkrzak, C.F. *et al*, *Phys. Rev. B*, 1982, **26**, 245 (*nd, struct*)
Shimotomai, M. *et al*, *Physica B+C (Amsterdam)*, 1985, **130**, 501 (*synth*)
King, R.B., *J. Solid State Chem.*, 1987, **71**, 233 (*struct*)
Hou, M.K. *et al*, *Solid State Commun.*, 1988, **65**, 895.

IC-001107

B_4O_5

Boron oxide (B_4O_5)

Boron suboxide

B_4O_5

M 123.2

Prepd. by evaporating a soln. of $H_2B_4O_5$ (obtained by hydrolysis of Mg_3B_2) *in vacuo*. White residue. Dissolves in H_2O to give $H_2B_4O_5$.

[54566-73-3]

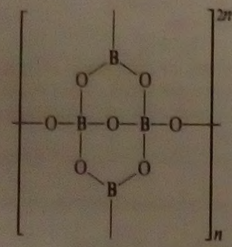
Ray, R.C. *et al*, *J. Chem. Soc.*, 1941, 742 (*synth*)

IC-001108

$B_4O_7^{2\ominus}$

Tetraborate(2−), 10CI, 9CI, 8CI

[12258-53-6]



M 155.2 (ion)

3D polyanion.

Di-Li salt: see *Lithium tetraborate, IC-001102*

Sr salt: [12007-66-8].

B_4O_7Sr M 242.8

Colourless cryst.

Lefebvre, J., *J. Chim. Phys. Phys.-Chim. Biol.*, 1957, **54**, 567 (*synth*)
Cuthbert, J.D. *et al*, *J. Chem. Phys.*, 1963, **38**, 1912 (*B-11 nmr*)
Perloff, A. *et al*, *Acta Crystallogr.*, 1966, **20**, 274 (*cryst struct*)
Krogh-Moe, J., *Acta Crystallogr., Sect. B*, 1968, **24**, 179 (*cryst struct*)
Farmer, J.B., *Adv. Inorg. Chem. Radiochem.*, 1982, **25**, 187 (*rev, bibl*)

B_4PrRh_4

IC-001109

Praseodymium rhodium boride ($PrRh_4B_4$), 10CI

[63100-10-7]

$PrRh_4B_4$

M 595.7

Possesses the $CeCo_4B_4$ struct. Superconducting below ~ 4.6K. Ferromagnetic. $\mu_{eff} = 3.10\mu_B$ (θ −2.6K); peak in heat capacity at 1.6K; below this temp. antiferromagnetic superconductor.

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*synth*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*struct*)
Dunlap, B.D. *et al*, *Solid State Commun.*, 1982, **44**, 1577 (*theory*)
Shimotomai, M. *et al*, *J. Less-Common Met.*, 1987, **135**, 161 (*synth, cond*)
Ooyama, T. *et al*, *Jpn. J. Appl. Phys., Part 1*, 1987, **26**, 1251 (*synth, cond*)
Ooyama, T. *et al*, *Physica B+C (Amsterdam)*, 1987, **148**, 133.

B_4ReSm

IC-001110

Rhenium samarium boride ($ReSmB_4$)

[84285-79-0]

$ReSmB_4$

M 379.8

Isostructural with $YCrB_4$. From phase equilibrium at 1000°.

Mikhalenko, S.I. *et al*, *Poroshk. Metall. (Kiev)*, 1982, 50; *CA*, **98**, 112030q (*synth, cryst struct*)

B_4ReTb

IC-001111

Rhenium terbium boride ($ReTbB_4$)

[12670-66-5]

$ReTbB_4$

M 388.3

Isostructural with $YCrB_4$.

Kuz'ma, Yu.B. *et al*, *Dopov. Akad. Nauk Ukr. RSR, Ser. A: Fiz. Mat. Tekh. Nauki.*, 1972, **34**, 166; *CA*, **76**, 132557r.

B_4ReTh

IC-001112

Rhenium thorium boride ($ReThB_4$)

[54065-39-3]

$ThReB_4$

M 461.4

Layer struct. of the $ThMoB_4$ kind. Isol. from the Th—Re—B phase system at 1750°.

Rogl, P. *et al*, *Monatsh. Chem.*, 1974, **105**, 1082 (*synth, cryst struct*)

B_4Re_4Y

IC-001113

Rhenium yttrium boride (Re_4YB_4)

[62339-31-5]

Re_4YB_4

M 876.9

Isostructural with $CeRe_4B_4$. From Y—Re—B system at 1000°.

Mikhalenko, S.I. *et al*, *Poroshk. Metall. (Kiev)*, 1977, 48; *CA*, **86**, 128127q.

B_4Rh_4Sm

IC-001114

Rhodium samarium boride (Rh_4SmB_4)

Samarium rhodium boride ($SmRh_4B_4$)

[62974-33-8]

$SmRh_4B_4$

M 605.2

Tetragonal phase is superconductor at low temps. (T_c ~2.5K); both ferromagnetic and antiferromagnetic phases are superconducting. Antiferromagnetic ordering occurs at 0.87K.

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1376 (*struct*)
Shirane, G. *et al*, *Bussei Kenkyu.*, 1981, **35**, 237 (*cond*)
Zasadzinski, J. *et al*, *Phys. Rev.*, 1984, **30**, 5095 (*magnetism*)
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)
Terris, B.D. *et al*, *Phys. Rev.*, 1986, **34**, 4868 (*magnetism*)
Noakes, D.R. *et al*, *Phys. Rev. B*, 1987, **35**, 6597 (*magnetism*)
Zhou, H. *et al*, *Phys. Rev. B*, 1987, **36**, 594 (*magnetic anisotropy*)
Hou, M.K. *et al*, *Solid State Commun.*, 1988, **65**, 895 (*cond*)

IC-001115

B_4Rh_4Tb

Rhodium terbium boride (Rh_4TbB_4)

Terbium rhodium boride ($TbRh_4B_4$)

[62974-34-9]

$TbRh_4B_4$

M 613.7

Ferromagnetic (T_c 7K). Hydrogenation catalyst for linear unsat. hydrocarbons.

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1335 (*magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1337 (*struct*)
Mackay, H.B. *et al*, *J. Low Temp. Phys.*, 1980, **41**, 639 (*magnetism*)
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)
Saito, K. *et al*, *J. Catal.*, 1987, **106**, 292 (*use*)
Japan. Pat., 62 221 447, (1987); *CA*, **109**, 8388 (*use*)

IC-001116

B_4Rh_4Tm

Rhodium thulium boride (Rh_4TmB_4)

Thulium rhodium boride ($TmRh_4B_4$)

[62974-36-1]

$TmRh_4B_4$

M 623.8

Tetragonal phase is superconductor; T_c ~9.6K. Metamagnetic transition at 0.49K. Spec. heat anomalies occur above T_c.

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*struct*)
Smith, J.L. *et al*, *J. Appl. Phys.*, 1979, **50**, 2330 (*props*)
Kuz'ma, Yu.B. *et al*, *J. Less-Common Met.*, 1979, **67**, 51 (*synth*)
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)
King, R.B., *J. Solid State Chem.*, 1987, **71**, 233 (*struct*)
Willekers, R.W., *Jpn. J. Appl. Phys., Part 1*, 1987, **26**, 1265 (*props*)
King, R.B., *Inorg. Chim. Acta*, 1988, **143**, 15.

B_4Rh_4Y

IC-001117

Rhodium yttrium boride (Rh_4YB_4)

Yttrium rhodium boride (YRh_4B_4)

[62974-37-2]

YRh_4B_4

M 543.7

Struct. based on a primitive tetragonal lattice with Rh_4B_4 cubes and Y atoms alternating. ($CeCo_4B_4$ type). Tetragonal phase is high-temp. superconductor; T_c ~11K. Superconductivity found also on partial subst. of Ru for Rh.

Matthias, B.T. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1334 (*magnetism*)
Vandenberg, J.M. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1977, **74**, 1336 (*cryst struct*)
Johnston, D.C., *Solid State Commun.*, 1977, **24**, 699 (*conductivity*)
Woolf, L.D. *et al*, *J. Low Temp. Phys.*, 1979, **35**, 651.
Lambert, S.E. *et al*, *Physica B+C (Amsterdam)*, 1985, **135**, 329 (*synth*)
Lee, W.H. *et al*, *J. Low Temp. Phys.*, 1987, **68**, 147.
King, R.B., *J. Solid State Chem.*, 1987, **71**, 233.

B_4Rh_4Yb

IC-001118

Rhodium ytterbium boride (Rh_4YbB_4)

Ytterbium rhodium boride ($YbRh_4B_4$)

[66506-05-6]

$YbRh_4B_4$

M 627.9

Pure phase not isolable; can be stabilised by incorporation of 15% Ru. Not superconducting above 1.5K.

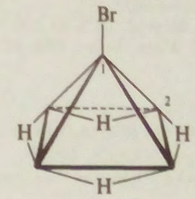
Johnston, D.C., *Solid State Commun.*, 1977, **24**, 699.
Delong, L.E. *et al*, *Ternary Supercond., Proc. Int. Conf., 1980*, Shenay, G.K. *et al*, Eds., Elsevier, 1981, 193.

B_5BrH_8

IC-001119

1-Bromopentaborane(9), 10CI

[23753-67-5]



M 142.0

nido-. Reactive compd. used for synthesis of other boranes. White solid. Mp 34°. Bp_{34} 82°.

▷ Spontaneously inflammable. Explosive with air.

Tucker, P. *et al*, *Inorg. Chem.*, 1970, **9**, 1430 (*nmr*)
Inorg. Synth., 1979, **19**, 247 (*synth, haz*)

$B_5CaH_{10}NaO_{14}$

IC-001120

Calcium sodium pentaborate pentahydrate

[12229-14-0]

$NaCa[B_5O_7(OH)_4].3H_2O$

M 351.1

Contains pentaborate chain polyanions (*cf.* Pentaborate(1−), IC-001126) linked through B—O—B bridges. Also formulated as $Na_2O.2CaO.5B_2O_3.10H_2O$. Used in production of fibreglass and borosilicate glasses. Colourless cryst. V. spar. sol. H_2O.

Mineral-form [12007-94-2]

Probertite, 10CI, 9CI

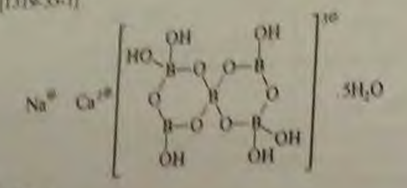
Occurs in assoc. with other borate minerals e.g. Colemanite. Brittle cryst.

Menzel, H. *et al*, *Z. Anorg. Allg. Chem.*, 1940, **245**, 157, 197 (*synth*)
Rumanova, I.M. *et al*, *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1966, **10**, 513 (*cryst struct*)
Menchetti, S. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 3072 (*cryst struct*)
Farmer, J.B. *et al*, *Therm. Anal., Proc. Int. Conf., 7th, 1982*, 1982, 650; *CA*, 1983, **99**, 168453 (*thermal anal*)

$B_5CaH_{10}NaO_{17}$ IC-001121

Calcium sodium pentaborate octahydrate

[1319-33-1]



M 405.2

Also formulated $NaCaB_5O_9.8H_2O$ or $Na_2O.2CaO.5B_2O_3.16H_2O$. Used in production of fibreglass and borosilicate glasses. Colourless solid. V. spar. sol. H_2O.

Mineral-form

Ulexite, 10Cl, 9Cl, Boronatrocalcite

Abundant in salt deposits of arid regions. Triclinic cryst. Loses $4H_2O$ on heating between 80-100°, a further 8.5 H_2O between 100-175° and the final $3.5H_2O$ at 450°.

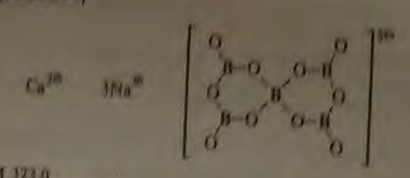
Kessans, A.D., *The Synth. of Borates in Aq. Solns. and their Investigation*, Akad. Nauk. Latv. S.S.S.R. Riga, 1955 (*synth*)
Clark, J.R. *et al, Am. Mineral.*, 1959, **44**, 712 (*cryst struct*)
Karazhanov, N.A. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1960, **11**, 747 (*thermal anal*)
Ghose, S. *et al, Am. Mineral.*, 1978, **63**, 160 (*cryst struct*)
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)

$B_5CaNa_2O_{10}$ IC-001122

Calcium sodium borate ($CaNa_2B_5O_{10}$)

Calcium trisodium pentaborate. Bis(μ-tetraoxotetraoxodiborato(4−))borate(5−), calcium sodium salt (1:1:3), 11Cl

[99230-74-7]



M 323.0

Struct. composed of polyanion with every O atom coordinating 1 to 4 cations $B_{tetrahedral}$–O 147, $B_{triangular}$–O_{cation} 139, $B_{triangular}$–O_{cation} 132 pm. Synth. by slow cooling of a melt of $Na_2O/CaO/B_2O_3$. Colourless solid.

Fayos, J. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 1396 (*synth, cryst struct*)

B_5ClH_8 IC-001123

1-Chloropentaborane(9), 10Cl

[19469-13-7]

M 97.5

nido- Colourless liq. or solid. Mp 27°.

Gaines, D. *et al, J. Am. Chem. Soc.*, 1966, **88**, 4528 (*ir*)
Gaines, D. *et al, Inorg. Chem.*, 1968, **7**, 704 (*synth*)
Tucker, P. *et al, Inorg. Chem.*, 1970, **9**, 1430 (*nmr*)
Murphy, C. *et al, Int. J. Mass Spectrom. Ion Phys.*, 1971, **7**, 327 (*ms*)

B_5ClH_8 IC-001124

2-Chloropentaborane(9), 10Cl

[19469-14-8]

M 97.5

nido- Colourless liq. Mp −41° (−40°).

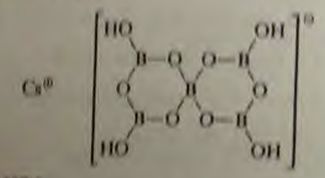
Gaines, D. *et al, Inorg. Chem.*, 1968, **7**, 704 (*synth*)
Burg, A., *J. Am. Chem. Soc.*, 1968, **90**, 1407 (*ir*)
Tucker, P. *et al, Inorg. Chem.*, 1970, **9**, 1430 (*nmr*)
Murphy, C. *et al, Int. J. Mass Spectrom. Ion Phys.*, 1971, **7**, 327 (*ms*)

$B_5CsH_8O_{12}$ IC-001125

Caesium pentaborate dihydrate

Dicaesium decaborate octahydrate. Caesium pentaborate tetrahydrate

[12229-10-6]



M 387.0

Also formulated $Cs_2O.5B_2O_3.8H_2O$. Colourless solid, α- and β-forms known. α-form dehydrates continuously up to 450°

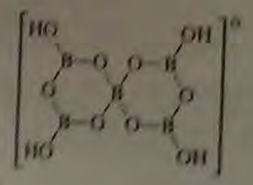
Kocher, J., *Bull. Soc. Chim. Fr.*, 1968, 919 (*synth*)
Benhassaine, A., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1933 (*thermal anal*)
Frohnecke, J. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 69 (*synth, ir*)
Behm, H., *Acta Crystallogr., Sect. C*, 1984, **40**, 1114 (*cryst struct*)

$B_5H_4O_{10}^{3\ominus}$ IC-001126

Pentaborate(1−)

Tetrahydrogen pentaborate, 9Cl. Borate (B_5O_{10})$^{5\ominus}$ tetrahydrogen, 8Cl

[12343-58-7]



M 218.6 (ion)

Na salt, trihydrate: see *Sodium pentaborate pentahydrate, IC-001134*

K salt, [14836-98-7].

$B_5H_4KO_{10}$ M 257.1

Colourless cryst. Sol. H_2O.

K salt, dihydrate: see *Potassium pentaborate dihydrate, IC-001129*

Rb salt, dihydrate: see *Rubidium pentaborate dihydrate, IC-001130*

Cs salt, dihydrate: see *Caesium pentaborate dihydrate, IC-001125*

NH_4 salt, dihydrate: see *Ammonium pentaborate tetrahydrate, IC-001137*

Ingri, N., *Acta Chem. Scand.*, 1963, **17**, 573, 581 (*synth*)
Krogh-Moe, *Acta Crystallogr., Sect. B*, 1972, **28**, 168 (*cryst struct*)
Devarajan, V. *et al, Spectrochim. Acta, Part A*, 1976, **32**, 1225 (*ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, 1977, **1**, 223 (*rev, lit*)
Janda, R. *et al, Z. Naturforsch., B*, 1979, **34**, 585, 1078 (*B-11 nmr, ir, raman*)

$B_5H_5^{2\ominus}$ IC-001127

Pentahydropentaborate(2−)

[12429-90-2]

proposed structure

M 59.0 (ion)

closo-: theoretical anion.

Kettle, S.F.A. *et al, J. Chem. Soc. A*, 1969, 2002.
Lipscomb, W.W. *et al, J. Am. Chem. Soc.*, 1977, **99**, 6226.
Olmare, B.M. *et al, J. Am. Chem. Soc.*, 1986, **108**, 4303.
Wade, K. *et al, Polyhedron*, 1986, **5**, 1437.

$B_5H_6^{\ominus}$ IC-001128

Octahydropentaborate(1−), 10Cl

M 62.1 (ion)

nido anion. Used for synthesis of other borane species.

K salt: [56009-95-1].

B_5H_9K M 101.2

Colourless cryst. Sol. Me_2O, Et_2O, glyme, THF.

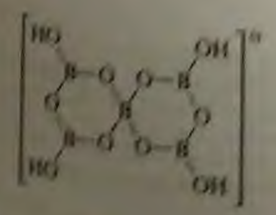
Johnson, H. *et al, Inorg. Chem.*, 1970, **4**, 908 (*synth, nmr, ir, cryst struct*)

$B_5H_8KO_{12}$ IC-001129

Potassium pentaborate dihydrate

Potassium pentaborate (KB_5O_8) tetrahydrate. Potassium tetrahydrogen borate(5−) dihydrate. Potassium tetrahydroxopentaborate dihydrate. Potassium dihydrogen dihydroxonium pentaborate. Boric acid (B_5HO_8), potassium salt, tetrahydrate, 8Cl. Boron potassium oxide (B_5KO_8) tetrahydrate, 11Cl, 10Cl, 9Cl

[37349-13-9]



M 309.2

Forms by reaction of boric acid (H_3BO_3) with KCl in a stream of steam. Used in fluxes for welding/brazing – shows interesting optical props. which make it suitable for use in dye lasers. Colourless orthorhombic cryst., α- and β-forms known, latter is metastable. Mod. sol. H_2O (2.4 g per 100 cm^3). Loses H_2O of crystallisation at 120-170°; becomes anhydrous at 440°.

Mineral-form [12360-03-1]

Santite

From Tuscany, Italy. Colourless cryst.

[64641-20-9]

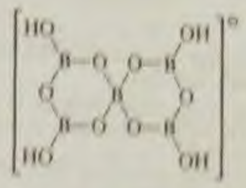
Hackspill, L. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1931, **192**, 48 (*synth*)
Zachariasen, W.H. *et al, Acta Crystallogr.*, 1963, **16**, 376 (*cryst struct*)
Furukawa, G.T. *et al, J. Res. Natl. Bur. Stand. (U.S.)*, 1964, **68A**, 381 (*thermodyn*)
Toledano, P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **271**, 1577 (*synth*)
Frey, K. *et al, Z. Naturforsch., B*, 1972, **27**, 101 (*ir*)
Cook, W.R. *et al, J. Opt. Soc. Am.*, 1976, **66**, 72 (*optical props*)
Janda, R. *et al, Z. Naturforsch., B*, 1979, **34**, 1078 (*B-11 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *Suppl.*, 1980, **1**, 236 (*uses*)
Voitsekhovskii, V.N. *et al, Kristallografiya*, 1982, **27**, 975 (*cryst struct*)
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)

$B_5H_8O_{12}Rb$ IC-001130

Rubidium pentaborate dihydrate

Dirubidium decaborate octahydrate. Rubidium pentaborate tetrahydrate

[37190-12-8]



M 339.5

Also formulated $Rb_2O.5B_2O_3.8H_2O$. Colourless cryst., α- and β-forms known. α-Form dehydrates continuously on heating.

Toledano, P., *Bull. Soc. Chim. Fr.*, 1966, 2302 (*synth*)
Benhassaine, A., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1933 (*synth, thermal anal*)
Behm, H., *Acta Crystallogr., Sect. C*, 1984, **40**, 217 (*cryst struct*)

$B_5H_9^{3\ominus}$ IC-001131

Pentaborate(9)(2−)

[108169-50-2]

M 63.1 (ion)

arachno-

Di-K salt:

$B_5H_9K_2$ M 141.3

Red-brown solid, dec. in air. Insol. pentane, THF, glyme.

Bis[(Kdibenzo-18-crown-6)] salt: Sol. THF, glyme.

Warren, J.R. *et al, Inorg. Chem.*, 1987, **26**, 1644 (*synth, ir, B-11 nmr*)

B_5H_9 IC-001132

Pentaborane(9), 10CT

[19624-22-7]

M 63.1
nido-. Stable intermed. used for prepn. of higher boranes. Many derivs. formed. Liq. Mp −46.6°. Bp 50.3°.

▷ Spontaneously inflammable (explosive) with air. Solvs. with reactive carbonyl groups and halogenated solvs. may form shock-sensitive solns. RY8925000

Dilcher, V. *et al*, *J. Res. Natl. Bur. Stand. (U.S.)*, 1949, **43**, 97 (*ms*)
McCarty, L. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 3138 (*synth*)
Hrostowski, H. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 998 (*ir*)
Onak, T., *J. Chem. Soc., Chem. Commun.*, 1972, 351 (*nmr*)
Inorg. Synth., 1974, **15**, 118 (*synth*)
Muetterties, E.L., *Boron Hydrides*, Academic Press, New York, 1975, 101 (*nmr*)

$B_5H_{10}LiO_{12}$ IC-001133

Lithium pentaborate pentahydrate

[37180-08-6]

$LiB_5O_8.5H_2O$

M 279.0
Struct. unknown; also formulated $Li_2O.5B_2O_3.10H_2O$.
Colourless solid. Sol. H_2O.

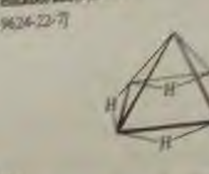
Reburn, W.T. *et al*, *J. Phys. Chem.*, 1955, **59**, 19 (*synth*)
Bendiamine, A., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C.*, 1972, **274**, 1358 (*synth*)
Nies, N.P., *Muller Compr. Treat. Inorg. Theor. Chem.*, Longmans, London, 1980, V/A, 347 (*rev*)

$B_5H_{10}NaO_{12}$ IC-001134

Sodium pentaborate pentahydrate

Sodium pentaborate trihydrate

[12046-75-2]



M 295.1
Also formulated $Na_2O.0.5B_2O_3.10H_2O$. Finds limited use in agriculture and in flame retardant formulations. Colourless cryst. Spar. sol. H_2O.

Mineral-form [39282-94-5]

Sborgite, 9CI

Occurs in association with other borate minerals and NaCl. Most common sodium pentaborate mineral. Colourless monoclinic cryst.

Nies, N.P. *et al*, *J. Chem. Eng. Data*, 1967, **12**, 303 (*synth*)
Merlino, S. *et al*, *Acta Crystallogr., Sect. B*, 1972, **32**, 3559 (*cryst struct*)
Janda, R. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 997 (*ir, raman*)

B_5H_{11} IC-001135

Pentaborane(11), 10CT

[18433-84-6]

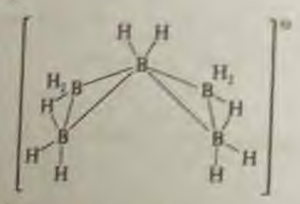
M 65.1
arachno-. Colourless liq. Mp −123°. Bp 63°.

Klein, M. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4149 (*synth*)
Lutz, C. *et al*, *Can. J. Chem.*, 1963, **41**, 1344 (*ms*)
Spielman, J. *et al*, *Inorg. Chem.*, 1963, **2**, 1139 (*ir*)
Feldner, T. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 381 (*ms*)
Leach, J.B. *et al*, *Inorg. Chem.*, 1970, **9**, 2170 (*nmr*)
Toft, M. *et al*, *Inorg. Chem.*, 1982, **21**, 1952 (*synth*)

$B_5H_{12}^{\ominus}$ IC-001136

Dodecahydropentaborate(1−), 9CT

[11056-98-7]



M 66.1 (ion)
hypho-. Proposed struct. shown. Synth. from KB_4H_9 and B_2H_6 in Et_2O at −35°.

Tetrabutylammonium salt: [57472-86-3].
Colourless cryst.

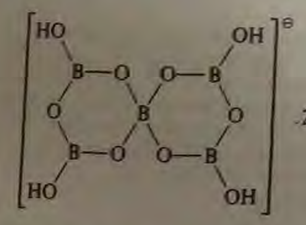
Ph_3PMe salt: [57472-88-5].
Colourless cryst.

Shore, S.G. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 3798; 1975, **97**, 5395; 1976, **98**, 449 (*synth, pmr, B-11 nmr*)

$B_5H_{12}NO_{12}$ IC-001137

Ammonium pentaborate tetrahydrate, 10CI

[12229-12-8]



M 272.1
Also formulated $(NH_4)B_5O_8.4H_2O$ or $(NH_4)_2O.5B_2O_3.8H_2O$. Used in flameproofing materials and in electrolytic capacitors. Has interesting optical props. Colourless cryst. known in α- and β-forms. Sol. H_2O. Loses H_2O more easily than NH_3 on heating. At 50° about 75% H_2O is lost compared to <1% NH_3.

Mineral-form

Larderellite

Has also been formulated $(NH_4)B_5O_6(OH)_4$. Occurs in boric acid lagoon at Larderello, Italy. Microscopic white cryst.

Tsiklauri, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C.*, 1968, **266**, 1155 (*synth*)
Jander, R. *et al*, *Z. Naturforsch., B*, 1979, **34**, 1078 (*B-11 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, Suppl., 1980, **1**, 236 (*synth*)
Jander, R. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 991 (*ir, raman*)
Dimitrievchev, M.V., *Acta Crystallogr., Sect. B*, 1981, **37**, 643 (*cryst struct*)
Solans, X. *et al*, *J. Appl. Crystallogr.*, 1983, **16**, 637 (*optical props*)

$B_5O_8^{\ominus}$ IC-001138

Pentaborate(5−), 10CI, 9CI

[60650-08-0]

$[B_5O_8]^{5\ominus}$

M 214.0 (ion)
May contain infinite chains of $(B_5O_{10})^{10\ominus}$ ions with three B atoms 4 coord., and two B atoms 3 coord.; or a layer struct. with 3 BO_4^- and 3 BO_3-groupings.

Ca(II), Sm(III) salt:
B_5CaO_8Sm M 423.3
Cryst.

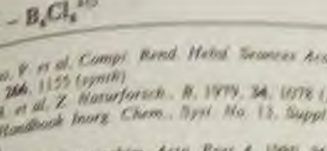
Ca(II), Ho(III) salt:
B_5CaHoO_8 M 437.9
Cryst.

Abdullaev, G.K. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1976, **17**, 961 (*cryst struct*)
Abdullaev, G.K. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 1286 (*cryst struct*)

B_6BeH_{14} IC-001139

[Decahydropentaborato(1−)][tetrahydroborato(1−)-*H,H*]beryllium, 10CI

[60923-64-0]



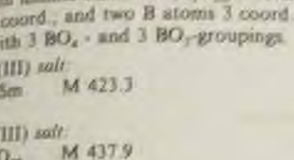
M 87.9
nido-. Liq. (by low temp. fractionation). Sol. C_6H_6. Mp −22°.

Gaines, D.F. *et al*, *Inorg. Chem.*, 1978, **17**, 1238, 1242 (*synth, ir, B-11 nmr, pmr, cryst struct*)
Bicerano, J. *et al*, *Inorg. Chem.*, 1979, **18**, 1565 (*theory*)
Gaines, D.F. *et al*, *J. Magn. Reson.*, 1981, **44**, 84 (*Be-9 nmr*)

B_6BrH_9 IC-001140

2-Bromohexaborane(10)

[50545-82-9]



M 153.8
nido-. Synth. from $B_6H_{10} + BBr_3$ at −45°. Also from $B_6H_{10} + Br_2$. Liq.

Shore, S.G. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6629.
Dolan, P.J. *et al*, *Inorg. Chem.*, 1981, **20**, 745 (*synth, B-11 nmr, ms*)

$B_6Br_6^{2\ominus}$ IC-001141

Hexabromohexaborate(2−), 11CI

X = Br

M 544.2 (ion)
closo-.

Di-Na salt: [95012-66-1].
$B_6Br_6Na_2$ M 590.2
Colourless cryst. (H_2O). Mod. sol. H_2O.

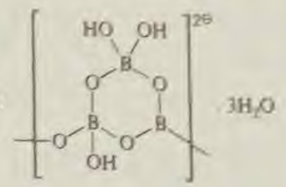
Bis-tetrabutylammonium salt: [95012-64-9].
Colourless cryst. (CH_2Cl_2/Et_2O). Sol. MeCN, CH_2Cl_2, Me_2CO; insol. H_2O. Hydrolytically stable.

Hertler, W.R. *et al*, *Chem. Eng. News*, 1966, **44**, 88 (*synth*)
Prentz, W. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1472 (*synth, ir, raman, B-11 nmr*)

$B_6CaH_{12}MgO_{17}$ IC-001142

Hydroboracite, 10CI, 9CI

[12046-12-7]



M 413.3
Contains infinite chains of $[B_3O_4(OH)_3]_n^{2n\ominus}$ anions. Also formulated $CaO.MgO.3B_2O_3.6H_2O$. Borate mineral - esp. important in USSR. Colourless cryst.

Kesans, A.D., *The Synth. of Borates in Aq. Soln. and their Investigation*, Akad. Nauk. Latv. SSR, Riga, 1955 (*synth, ir, optical props*)
Rumanova, I.M. *et al*, *Kristallografiya*, 1963, **8**, 828 (*cryst struct*)
Rumanova, I.M. *et al*, *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1963/4, **8**, 665 (*cryst struct*)
Karazhanov, N.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1966, **11**, 747 (*thermal anal*)
Rza-Zade, P.F. *et al*, *CA*, 1972, **77**, 83030.

$B_6Cl_6^{2\ominus}$ IC-001143

Hexachlorohexaborate(2−), 11CI, 9CI

[39343-09-4]

As Hexabromohexaborate(2−), IC-001141 with

X = Cl

M 277.5 (ion)
closo-.

Di-Cs salt: [95012-67-2].
$B_6Cl_6Cs_2$ M 543.3
Colourless cryst. (H_2O). Sol. H_2O.

Bis-tetrabutylammonium salt: [94191-06-7].

Colourless cryst. (CH_2Cl_2/Et_2O). Sol. MeCN, CH_2Cl_2, Me_2CO; insol. H_2O. Hydrolytically stable.

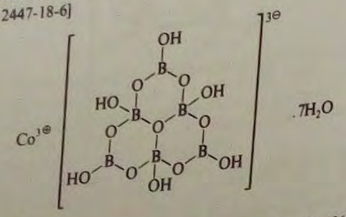
Preetz, W. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1472 (*synth, ir, raman, B-11 nmr*)

IC-001144

$B_6CoH_{20}O_{20}$

Cobalt(*III*) hexaborate decahydrate

[12447-18-6]



M 463.9

Shchigol, M.B. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1961, **6**, 1361 (*synth*)

Silins, E. *et al*, *CA*, 1973, **78**, 37308 (*cryst struct*)

Svarcs, E. *et al*, *CA*, 1973, **78**, 90573 (*ir*)

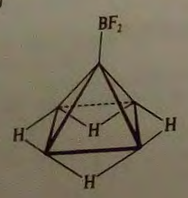
Svarcs, E. *et al*, *Proc. Eur. Symp. Therm. Anal., 1st*, 1976, 291.

IC-001145

$B_6F_2H_8$

1-(Difluoroboryl)pentaborane(9)

[120385-36-6]



M 110.9

nido-. Colourless liq. Sol. CH_2Cl_2.

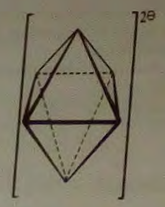
Saulys, D.A. *et al*, *Inorg. Chem.*, 1989, **28**, 1619 (*synth, pmr, B-11 nmr, F-19 nmr, ms*)

IC-001146

$B_6H_6^{2\ominus}$

Hexahydrohexaborate(2–), 9CI

[12429-97-9]



M 70.9 (ion)

closo-. Synth. from B_2H_6 and $NaBH_4$ in diglyme at 100°. Reflux at 162° for 16.5 hrs. Salts sol. H_2O; insol. Et_2O.

Bis-Me_4N salt: Solid. Mp >300°.

Boone, J.L., *J. Am. Chem. Soc.*, 1964, **86**, 5036 (*synth, derivs, B-11 nmr, ir*)

Schaeffer, R. *et al*, *Inorg. Chem.*, 1965, **4**, 917 (*powder struct, Me_4N salt*)

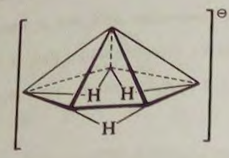
Muetterties, E.L. *et al*, *Inorg. Chem.*, 1967, **6**, 1271 (*synth*)

IC-001147

$B_6H_9^{\ominus}$

Nonahydrohexaborate(1–), 10CI

[31426-85-4]



M 73.9 (ion)

*nido-*anion.

K salt:

B_6H_9K M 113.0

Colourless cryst., unstable at r.t. Sol. ethers.

Johnson, H. *et al*, *Inorg. Chem.*, 1970, **9**, 908 (*synth, cryst struct, nmr*)

Johnson, H. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 6711 (*pmr, ir*)

IC-001148

B_6H_{10}

Hexaborane(10)

[23777-80-2]

M 74.9

nido-. Liq. Mp −62.3°. Bp 108°.

Bis-Me_3N complex:

$C_6H_{28}B_6N_2$ M 193.1

Bis-Me_3P complex: see *Hexaborane(10) bis(trimethylphosphine), IC-005550*

Rossmann, M.G. *et al*, *Acta Crystallogr.*, 1959, **12**, 530 (*cryst struct*)

Shapiro, I. *et al*, *Adv. Chem. Ser.*, 1961, **32**, 127 (*ms*)

Burg, A.B. *et al*, *Inorg. Chem.*, 1962, **1**, 725 (*ir*)

Leach, J.B. *et al*, *Inorg. Chem.*, 1970, **9**, 2170 (*nmr*)

Brice, V. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6629 (*nmr*)

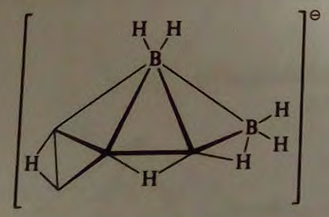
Inorg. Synth., 1979, **19**, 247 (*synth*)

IC-001149

$B_6H_{11}^{\ominus}$

Undecahydrohexaborate(1–), 11CI, 9CI, 8CI

[12430-03-4]



M 75.9 (ion)

arachno-.

K salt: [57406-40-3].

$B_6H_{11}K$ M 115.0

Sol. Me_2O. Stable at r.t. for approx. 1 h.

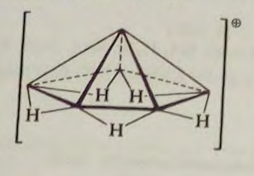
Tetrabutylammonium salt: More stable than K salt.

Remmel, R.J. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 5395 (*synth, pmr, B-11 nmr*)

$B_6H_{11}^{\oplus}$

Undecahydrohexaboron(1+), 9CI

IC-001150



M 75.9 (ion)

nido-.

Tetrachloroborate(1–): [37336-17-7].

$B_7Cl_4H_{11}$ M 228.5

Colourless solid, dec. at −40°. Sol. CH_2Cl_2.

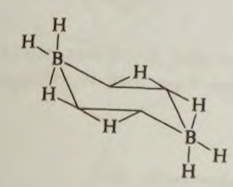
Johnson, H.D. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 6711 (*synth, pmr, B-11 nmr, raman*)

B_6H_{12}

Hexaborane(12), 10CI

IC-001151

[12008-19-4]



M 76.9

arachno-. Colourless liq., dec. slowly at 25°. Mp −82°. Bp 80-90°.

Gaines, D. *et al*, *Inorg. Chem.*, 1964, **3**, 438 (*synth, ir*)

Leach, J.B. *et al*, *Inorg. Chem.*, 1970, **9**, 2170 (*nmr*)

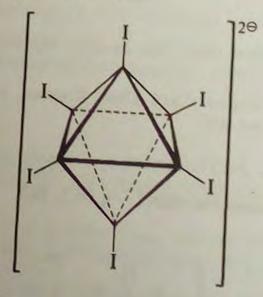
Remmel, R. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 3798 (*synth*)

McLaughlan, E. *et al*, *J. Phys. Chem.*, 1971, **75**, 3106 (*ms*)

$B_6I_6^{2\ominus}$

Hexaiodohexaborate(2–)

IC-001152



M 826.2 (ion)

closo- Octahedral B_6 cluster.

Di-Cs salt: [95012-72-9].

$B_6Cs_2I_6$ M 1092.1

Colourless cryst. (H_2O). Spar. sol. H_2O.

Bis-tetrabutyammonium salt: [95012-70-7].

Colourless cryst. (CH_2Cl_2/Et_2O). Sol. Me_2CO, MeCN, CH_2Cl_2; insol. H_2O. Hydrolytically stable.

Preetz, W. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1472 (*synth, ir, raman, B-11 nmr*)

B_6O

Boron oxide (B_6O), 11CI, 10CI, 9CI, 8CI

IC-001153

Hexaboron monoxide. Boron suboxide

[11056-99-8]

M 80.8

The boron sub-oxides whose separate existences have been questioned are listed here. For other sub-oxides, see e.g. Boron oxide (BO), IC-000907 and Boron oxide (B_2O_2), IC-001010. Sol. strong oxidising acids eg. HNO_3, $HClO_4$. Isostructural with α-B_n.

***Boron oxide* ($B_{12}O_2$)** [54723-68-1]

$B_{12}O_2$ M 161.7

Reddish-brown powder. Sol. conc. HNO_3. Dec. >1760 to B + O_2.

***Boron oxide* ($B_{13}O_2$)** [56940-67-1]

$B_{13}O_2$ M 172.5

Isostructural with α-B_n.

***Boron oxide* (B_7O)** [12447-73-3]

Heptaboron monoxide

B_7O M 91.6

Brown microcryst.

Pasternak, R.A., *Acta Crystallogr.*, 1959, **12**, 612 (*synth, powder struct, B_7O*)

Rizzo, H.F. *et al*, *J. Electrochem. Soc.*, 1962, **109**, 1079 (*synth, $B_{12}O_2$*)

U.S. Pat., 3 660 031, (1970/2); *CA*, 1972, **77**, 37152 (*B_7O*)

Petrak, D.R. *et al*, *NBS Spec. Publ. (U.S.)*, 1972, **364**, 605; *CA*, 1972, **27**, 157316 (*synth, raman, B_6O, $B_{12}O_2$*)

Jean-Blain, H. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1973, **277**, 977 (*synth, B_7O*)

Petrak, D.R. *et al*, *Am. Ceram. Soc. Bull.*, 1974, **53**, 569 (*synth, props, B_6O,$B_{13}O_2$, $B_{12}O_2$*)

Becher, H.J. *et al*, *Z. Anorg. Allg. Chem.*, 1974, **410**, 274 (*ir, B_6O, $B_{12}O_2$*)

Bills, P.M. *et al*, *J. Less-Common Met.*, 1976, **45**, 343 (*powder struct, $B_{12}O_2$*)

Domashevskaya, E.P. *et al*, *J. Less-Common Met.*, 1976, **47**, 189 (*pe, $B_{13}O_2$*)

Karpinos, D.M. *et al*, *CA*, 1983, **99**, 98230 (*synth, B_7O*)

Ugai, Yu.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 753 (*synth, B_6O*)

Brodhag, C. *et al*, *J. Less-Common Met.*, 1986, **117**, 1 (*synth, $B_{12}O_2$*)

$B_6O_{12}^{6\ominus}$

Hexaborate(6–)

IC-001154

$[B_6O_{12}]^{6\ominus}$

M 256.8 (ion)

Polymeric anion: can have all BO_4 groups linked to give a 3D array or 4 BO_4 and2 BO_3 units.

Tri-Ca salt: Calcium hexaborate (anhydr.) ($Ca_3B_6O_{12}$)

$B_6Ca_3O_{12}$ M 377.0

Colourless cryst.

$(Zn_4O)^{6\oplus}$ salt: [12008-25-2]. *Zinc hexaborate oxide* ($Zn_4(B_6O_{12})O$)

$B_6O_{13}Zn_4$ M 534.4

Colourless cryst.

Chang, C.H. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 378 (*synth, ir*)

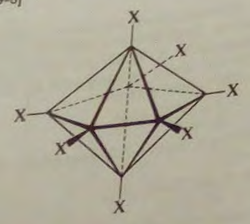
Marezio, M. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 955 (*cryst struct*)

Bondareva, O.S. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1978, **241**, 815 (*synth*)

Murray, A.F. *et al*, *J. Phys. C*, 1978, **11**, 387 (*raman*)

Smith-Verdier, P. *et al*, *Z. Kristallogr.*, 1980, **151**, 175 (*cryst struct*)

B_7Br_7 IC-001155
Heptabromoheptaborane(7), 11CI
Boron bromide (B_7Br_7), 10CI, 8CI
[12589-29-6]



X = Br

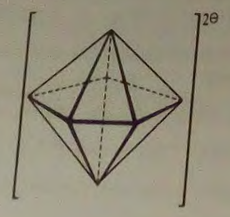
M 635.0
Moisture sensitive black solid. Sol. BBr_3. Thermally stable to 250° *in vacuo*. Dec. to B_9Br_9.
Kane, J. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 1195 (*synth, ms*)
Kutz, N.A. *et al*, *Inorg. Chem.*, 1980, **19**, 3295 (*synth, ms, B-11 nmr*)

$B_7ClMn_3O_{13}$ IC-001156
Manganese boracite, 11CI
Chambersite
[12418-60-9]

$Mn_3(B_7O_{13})Cl$

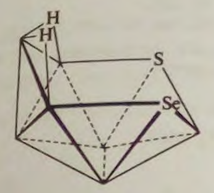
M 483.9
The Mn boracites $Mn_3B_7O_{13}X$ (X = halide, OH, S, Se, Te) belong to an extensive class of compds. Prepd. from MnO, $MnCl_2$ and B_2O_3 by vapour transport method or by melting the components together. Mineral of the boracite ($Mg_3B_7O_{13}Cl$) group. Colourless to deep purple cryst. Structure assumed to be similar to $Mg_3B_7O_{13}Cl$ with a cubic lattice. At 680 K undergoes phase transition to ferroelectric orthorhombic phase. $\mu_{eff} = 5.78\mu_B$. T_N 5K.
Honea, R.M. *et al*, *Am. Mineral.*, 1962, **47**, 665 (*props*)
Schmid, H. *et al*, *J. Phys. Chem. Solids*, 1965, **26**, 973 (*synth, struct*)
Fouassier, C. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **375**, 202 (*synth*)
Levasseur, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1973, **277**, 421 (*magnetism*)
Schmid, H. *et al*, *Ferroelectrics*, 1978, **20**, 21 (*phase transitions, optical props*)
Lockwood, D.J., *Indian J. Pure Appl. Phys.*, 1978, **16**, 268 (*optical props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 92 (*rev, bibl*)

$B_7H_7^{2\ominus}$ IC-001157
Heptahydroheptaborate(2−)
[12430-07-8]



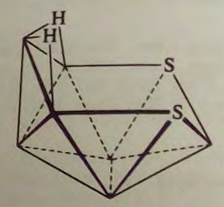
M 82.7 (ion)
closo-. Least stable of the $[B_nH_n]^{2\ominus}$ species.
Di-Cs salt:
$B_7Cs_2H_7$ M 348.5
Colourless solid. Sol. H_2O; insol. Et_2O, MeOH.
Klanberg, F. *et al*, *Inorg. Chem.*, 1967, **6**, 1271 (*synth, uv, ir, B-11 nmr*)

B_7H_9SSe IC-001158
5-Thia-9-selenanonaborane(9), 10CI
5-Selena-9-thianonaborane(9)
[72214-09-6]



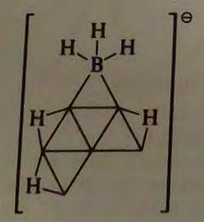
M 195.7
arachno-. Yellow solid. Sol. hexane. Mp 115-120° dec.
Friesen, G.D., *Inorg. Chem.*, 1980, **19**, 458 (*synth, ir, B-11 nmr, ms*)

$B_7H_9S_2$ IC-001159
5,9-Dithianonaborane(9), 10CI
[63115-77-5]



M 148.8
nido-. Pale-yellow cryst. Sol. hexane. Mp 103°. Subl. $_{0.01}$ 50°.
Plešek, J. *et al*, *Collect. Czech. Chem. Commun.*, 1977, **42**, 785 (*synth, nmr, ms, uv*)

$B_7H_{12}^{\ominus}$ IC-001160
Dodecahydroheptaborate(1−), 9CI, 8CI
[12430-09-0]

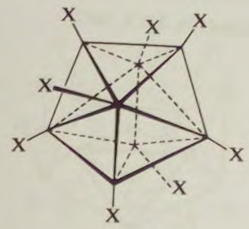


M 87.7 (ion)
arachno-.
K salt:
$B_7H_{12}K$ M 126.4
Sol. CH_2Cl_2. Dec. at r.t.
Tetrabutylammonium salt: [57298-54-1].

Sol. CH_2Cl_2. Dec. at r.t.
Remmel, R.J. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 5395 (*synth, pmr, B-11 nmr*)

B_7H_{13} IC-001161
Heptaborane(13), 11CI, 9CI, 8CI
[12008-34-3]
M 88.7
arachno - but detailed struct. unknown. Not isol. - ms evidence only.
Fehlner, T.P. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1012 (*ms*)
Bayliss, A.B. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 929 (*ms*)

B_8Br_8 IC-001162
Octabromooctaborane(8), 11CI
Boron bromide (B_8Br_8), 10CI, 8CI. Octaboron octabromide
[12589-30-9]



X = Br

M 725.7
Air- and moisture-sensitive dark red-brown solid. Sol. halogenated solvs. Dec. at 200° *in vacuo* to B_9Br_9.
Kutz, N.A. *et al*, *Inorg. Chem.*, 1980, **19**, 3295 (*synth, ms, B-11 nmr*)
Markwell, A. *et al*, *Polyhedron*, 1982, **1**, 134 (*synth, ms*)

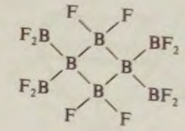
B_8Cl_8 IC-001163
Octachlorooctaborane(8), 11CI
Boron chloride (B_8Cl_8), 8CI. Octaboron octachloride
[32915-80-3]

As Octabromooctaborane(8), IC-001162 with

X = Cl

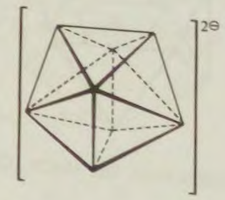
M 370.1
Air- and moisture-sensitive purple or dark red solid. Sol. BCl_3, CH_2Cl_2. Mp 185° (sealed tube). Dec at 200° to B_9Cl_9.
Jacobsen, R.A. *et al*, *J. Chem. Phys.*, 1959, **31**, 605 (*cryst struct*)
Lanthier, G.F. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 1569 (*synth, uv, ir, ms*)
Emery, S. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 6790 (*synth, B-11 nmr*)

B_8F_{12} IC-001164
1,1,3,3-Tetrakis(difluoroboryl)-2,2,4,4-tetrafluorotetraborane(8), 9CI
Dodecafluorooctaborane(12)
[39114-22-2]



M 314.4
Pale yellow in solid state – yellow, oily volatile liq. unstable at r.t. Dec. rapidly in gas phase. Sol. CH_2Cl_2.
▷ Reacts explosively with air or water.
Timms, P.L., *J. Am. Chem. Soc.*, 1967, **89**, 1629 (*synth*)
Kirk, R.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1392 (*synth, ir, ms, B-11 nmr, F-19 nmr, uv*)
Timms, P.L., *Acc. Chem. Res.*, 1973, **6**, 118 (*rev*)

$B_8H_8^{2\ominus}$ IC-001165
Octahydrooctaborate(2−), 11CI, 10CI, 9CI, 8CI
[12430-13-6]



M 94.5 (ion)
closo-.
Di-Cs salt: [12421-61-3].
$B_8Cs_2H_8$ M 360.3
Colourless cryst. (H_2O). Sol. H_2O. Stable up to 600° in sealed tube.
Tetraamminezinc(2+) salt: [12421-62-4].
$B_8H_{20}N_4Zn$ M 228.0
Colourless cryst. (aq. NH_3). Sol. H_2O.
Klanberg, F. *et al*, *Inorg. Chem.*, 1967, **6**, 1271 (*synth, uv, ir, B-11 nmr, electrochem*)
Inorg. Synth., 1968, **11**, 24 (*synth, uv, ir*)
Guggenberger, L.J., *Inorg. Chem.*, 1969, **8**, 2771 (*cryst struct*)
Muetterties, E.L. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 7520 (*synth, B-11 nmr*)

$B_8H_8Na_2O_{17}$ IC-001166
Disodium octaborate tetrahydrate
Polybor(60). Boron sodium oxide ($B_8Na_2O_{13}$), tetrahydrate, 11CI, 10CI, 9CI
[12280-03-4]

$Na_2O.4B_2O_3.4H_2O$

M 412.5
A commercially available sodium borate hydrate whose composition corresp. closely to the formulation of the hypothetical compd. Produced from mixtures of borax and boric acid. Used in wood preservatives, fertiliser sprays, herbicides, fire retardants. V. sol. H_2O.
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 84 (*soly, formulation*)
Nies, N.P., *Mellor Compr. Treat. Inorg. Theor. Chem.*, Longman, London, 1980, **V/A**, 343.

IC-001167

$B_8H_{10}S$
7-Thianonaborane(10), 9CI
4-Thianonaborane(10)
[59351-07-4]

M 128.6
nido-. Colourless solid, air- and water-sensitive. Sol. C_6H_6, CH_2Cl_2, pet. ether. Subl. 40° *in vacuo*. Stored at −78°.

Pretzer, W. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1441 (*synth, nmr, ir, ms*)

IC-001168

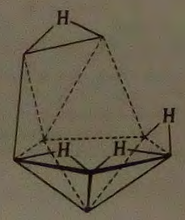
$B_8H_{10}Se_2$
6,9-Diselenadecaborane(10), 10CI
[69550-87-4]

M 254.4
arachno-. Colourless cryst. Sol. MeCN, $CHCl_3$. Mp 197-199° dec.

Friesen, G.D. *et al*, *Inorg. Chem.*, 1980, **19**, 1485 (*synth, ir, B-11 nmr, ms*)

IC-001169

B_8H_{12}
Octaborane(12), 10CI

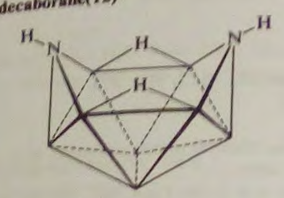


M 98.5
nido-, but exhibits more open *arachno*-structure. Sol. pentane. Mp −20°. Unstable above Mp.

Enrione, R. *et al*, *Inorg. Chem.*, 1964, **3**, 1659 (*cryst struct*)
Dobson, J. *et al*, *Inorg. Chem.*, 1968, **7**, 402 (*synth*)
Steck, *et al*, *Inorg. Chem.*, 1970, **9**, 2452 (*ms*)
Rietz, R. *et al*, *Inorg. Chem.*, 1972, **11**, 1242 (*nmr*)

IC-001170

$B_8H_{12}N_2$
6,9-Diazadecaborane(12)

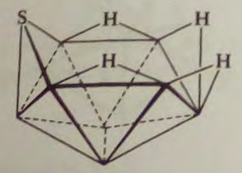


M 126.5
arachno-. Colourless solid. Sol. hexane, THF. Mp 23°. Unstable on prolonged exposure to air.

Stibr, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1990, 1309 (*synth, pmr, B-11 nmr, ms*)

IC-001171

$B_8H_{12}S$
4-Thianonaborane(12), 11CI, 10CI
[73711-47-4]

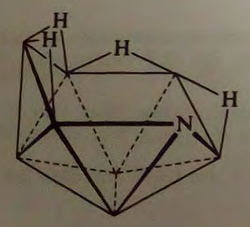


M 130.6
arachno-. Yellow solid; has limited stability in air. Sol. org. solvs. Dec. on heating.

Pretzer, W.R. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1441 (*synth, ir, B-11 nmr*)
Base, K. *et al*, *Chem. Ind. (London)*, 1979, 743 (*synth, pmr, B-11 nmr, ms*)
Dolansky, J. *et al*, *Collect. Czech. Chem. Commun.*, 1981, **46**, 2479 (*B-11 nmr*)
Base, K., *Collect. Czech. Chem. Commun.*, 1983, **48**, 2593 (*synth, pmr, B-11 nmr*)
Kang, S.O. *et al*, *Inorg. Chem.*, 1988, **27**, 3298 (*synth*)

IC-001172

$B_8H_{13}N$
4-Azanonaborane(13), 10CI
[58920-21-1]

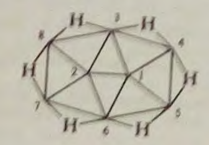


M 113.5
Air-sensitive liq. Sol. C_6H_6. Mp 0°. $Bp_{0.01}$ 60°.

Base, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 934 (*synth, ir, struct*)

B_8H_{14}
Octaborane(14), 10CI, 9CI, 8CI
[12008-46-7]

IC-001173

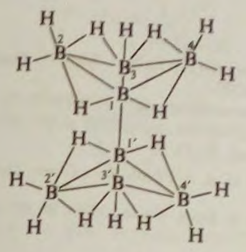


M 100.5
Colourless solid, unstable at r.t. Sol. pentane, CS_2.

Dobson, J. *et al*, *Inorg. Chem.*, 1968, **7**, 402 (*synth, B-11 nmr*)
Moody, D.C. *et al*, *Inorg. Chem.*, 1976, **15**, 233 (*pmr, B-11 nmr*)

B_8H_{18}
1,1′-Bitetraborane(10), 11CI
1′-(1-Tetraboran(10)yl)tetraborane(10). Octaborane(18), 9CI, 8CI

IC-001174



M 104.6
commo-(*conjuncto*) with two *arachno*-B_4H_9 residues.
[12421-66-8]

Steck, S.J. *et al*, *Inorg. Chem.*, 1969, **8**, 830 (*synth*)
Rietz, R.R. *et al*, *Inorg. Chem.*, 1972, **11**, 1242 (*synth*)
Corcoran, E.W. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 7793 (*synth, pmr, B-11 nmr*)

B_8H_{18}
2,2′-Bitetraborane

IC-001175

2-(2′-Tetraboran-10-yl)tetraborane(10). Octaborane(18)
[12421-66-8]
M 104.6
2,2-Linked *arachno-*. Thermally unstable.

Steck, S. *et al*, *Inorg. Chem.*, 1969, **8**, 830 (*ms*)
Rietz, R.R. *et al*, *Inorg. Chem.*, 1972, **11**, 1242 (*nmr*)
Glore, J. *et al*, *Inorg. Chem.*, 1973, **12**, 2175 (*synth*)

$B_8H_{32}Zn_3^{2\ominus}$
Octakis(tetrahydroborato)trizincate(2−)
Octakis(borohydrido)trizincate(2−)

IC-001176

$[Zn_3(BH_4)_8]^{2\ominus}$

M 314.9 (ion)
Di-K salt: [55965-48-5]. *Potassium zinc borohydride*
$B_8H_{32}K_2Zn_3$ M 393.1
From $ZnCl_2$ and KBH_4 in Et_2O at 0°. Cryst. (Et_2O). Sol. Et_2O (2.7 g in 100g at 0°). Dec. at 60°.
▷ Ignites spontaneously in air and on reaction with H_2O.
[20393-67-3]

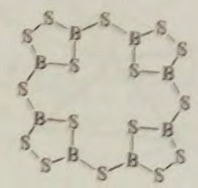
Hagemüller, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **248**, 2758 (*synth, ir, powder struct*)

Mikheeva, V.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 682 (*synth, ir, powder struct, thermal anal*)
Mal'tseva, N.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 363; 1975, **20**, 339 (*synth, powder struct, ir*)

B_8S_{16}
Boron sulfide (BS_2)

IC-001177

2,4,5,7,9,10,12,14,15,17,19,20,21,22,23,24-Hexadecathia-1,3,6,8,11,13,16,18-octaborapentacyclo[16.2.1.1^{3,6}.1^{8,11}.1^{13,16}]tetracosane, 9CI
[73825-17-9]

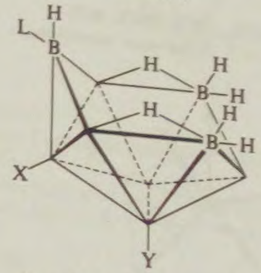


M 599.5
An 'inorganic porphyrin'. Synth. from B_2S_3 + S at 300°. Colourless moisture-sensitive cryst. Mp 115° dec.
[12045-25-9]

Krebs, B. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1980, **19**, 481; 1983, **22**, 113 (*synth, cryst struct*)
Gimarc, B.M. *et al*, *Inorg. Chem.*, 1982, **21**, 21; 1983, **22**, 479 (*electronic struct*)

B_9BrH_{12}
1-Bromononaborane(13)

IC-001178



Me_2S complex

L = SMe_2, X = Br, Y = H

M 189.2
Obt. as complexes which have *arachno*-struct.
Me_2S complex: [32357-04-3]. *4-(Dimethyl sulfide)-1-bromononaborane(13)*
$C_2H_{18}B_9BrS$ M 251.4
Colourless cryst. Sol. CH_2Cl_2, Me_2CO. Mp 123-125°.

Bodner, B.M. *et al*, *Inorg. Chem.*, 1971, **10**, 942 (*synth, B-11 nmr*)

$B_9Br_2H_{11}$
Dibromononaborane(13)

IC-001179

As 1-Bromononaborane(13), IC-001178 with

L = SMe_2, X = Y = Br

M 268.1
nido-B_9 cage. Several possible isomers.
Me_2S complex: [26162-05-0]. *4-(Dimethyl sulfide)-1,2-dibromononaborane(13)*
$C_2H_{17}B_9Br_2S$ M 330.3

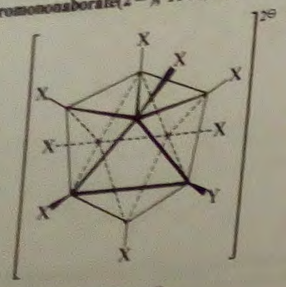
Colourless cryst. (CH_2Cl_2/Et_2O). Sol. C_6H_6, CH_2Cl_2. *arachno*. Loses H_2 at 91° in sealed tube - does not melt below 180°.

Stibr, B. *et al, Collect. Czech. Chem. Commun.*, 1969, **34**, 3241 (*synth, ir*)

IC-001180

$B_9Br_9^{2\ominus}$

Nonabromononaborate(2−), 11Cl, 10Cl



X = Y = Br

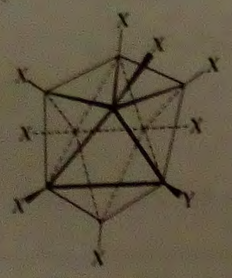
M 816.4 (ion)
closo-.
Bis-tetrabutylammonium salt: [72402-95-0].
Colourless cryst. (Me_2CO/hexane). Sol. CH_2Cl_2, MeCN.

Wong, E.H. *et al, Inorg. Chem.*, 1980, **19**, 451 (*synth, uv, ir, B-11 nmr*)

IC-001181

B_9Br_9

Nonabromononaborane(9), 11Cl, 10Cl, 9Cl
Boron bromide (B_9Br_9), 8Cl. Nonaboron nonabromide
[12589-31-0]



X = Y = Br

M 816.4
closo-. Product of thermal dec. of B_5Br_7 and B_9Br_{13}. Dark red cryst. (BBr_3); bright yellow vapour. Sol. BBr_3, CCl_4, CH_2Cl_2. Stable for 1 hr. in contact with H_2O. Thermally stable to 250° *in vacuo*. Subl. before melting.

Reason, M.S. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 1593 (*synth, ir, ms, uv*)
Wong, E.H. *et al, Inorg. Chem.*, 1980, **19**, 451 (*synth*)
Kutz, N.A. *et al, Inorg. Chem.*, 1980, **19**, 3295 (*synth, ms, B-11 nmr*)

B_9Cl_9H

IC-001182

Octachlorononaborane(9), 11Cl, 10Cl
[72275-11-7]

As Nonabromononaborane(9), IC-001181 with

X = Cl, Y = H (position undetermined)

M 381.9
Volatile yellow-orange solid (red cryst.); readily hydrol. Sol. hexane. Mp 224-225°.

▷ Pyrophoric.

Forstner, J.A. *et al, Inorg. Chem.*, 1964, **3**, 155 (*synth, uv, ir, ms, B-11 nmr*)
Reason, M.S. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 1593 (*synth, ms*)
Wong, E.H. *et al, Inorg. Chem.*, 1980, **19**, 451 (*synth*)
Saulys, D.A. *et al, Inorg. Chem.*, 1983, **22**, 1821 (*synth, ms, B-11 nmr*)

IC-001183

$B_9Cl_9^{2\ominus}$

Nonachlorononaborate(2−), 11Cl, 10Cl
[68517-22-6]

As Nonabromononaborate(2−), IC-001180 with

X = Y = Cl

M 416.3 (ion)
closo-.
Di-Na salt:
$B_9Cl_9Na_2$ M 462.3
Colourless solid (H_2O). Sol. MeCN. Stable to 12*M* HCl and 6*M* NaOH.
Bis-tetrabutylammonium salt: [68694-93-9].
Air and H_2O stable colourless solid. Sol. CH_2Cl_2, MeCN; insol. Et_2O.

Kabbani, R.M. *et al, J. Chem. Soc., Chem. Commun.*, 1978, 462 (*synth*)
Wong, E.H. *et al, Inorg. Chem.*, 1980, **19**, 451 (*synth, uv, ir, B-11 nmr*)

IC-001184

B_9Cl_9

Nonachlorononaborane(9), 11Cl, 10Cl
Boron chloride (B_9Cl_9), 8Cl. Nonaboron nonachloride
[12008-47-8]

As Nonabromononaborane(9), IC-001181 with

X = Y = Cl

M 416.3
Yellow-orange cryst. Sol. BCl_3, chlorinated hydrocarbons. Mp >350°.

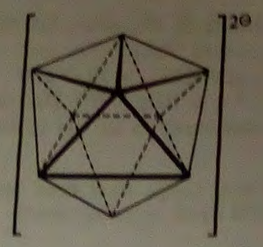
[31304-34-4]

Lanthier, G.F. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 1807 (*synth, uv, ir, ms, B-11 nmr*)
Hursthouse, M.B. *et al, Nature (London)*, 1970, **228**, 659 (*cryst struct*)
Kabbani, R.M. *et al, J. Chem. Soc., Chem. Commun.*, 1978, 462 (*synth*)
Wong, E.H. *et al, Inorg. Chem.*, 1980, **19**, 451; 1981, **20**, 1300 (*synth, uv, ir*)

IC-001185

$B_9H_9^{2\ominus}$

Nonahydrononaborate(2−), 11Cl, 10Cl, 9Cl, 8Cl
[12430-24-9]



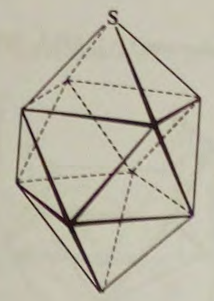
M 106.3 (ion)

closo-.
Di-Cs salt: [12046-61-6].
$B_9Cs_2H_9$ M 372.1
Colourless cryst. (hot H_2O). Sol. H_2O, MeCN; unstable in aq. acid solns.

Klanberg, F. *et al, Inorg. Chem.*, 1966, **5**, 1955 (*synth, uv, ir, raman, B-11 nmr*)
Guggenberger, L.J., *Inorg. Chem.*, 1968, **7**, 2260 (*cryst struct*)
Inorg. Synth., 1968, **11**, 27 (*synth, uv, ir*)
Carter, J.C. *et al, Inorg. Chem.*, 1970, **9**, 1777 (*synth*)
Muetterties, E.L. *et al, Inorg. Chem.*, 1975, **14**, 950 (*B-11 nmr*)

B_9H_9S

1-Thiadecaborane(9) IC-001186
[41646-56-4]

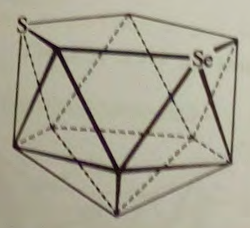


M 138.4
closo-. White cryst. by subl. *in vacuo*. Mp 216.5° (sealed tube).

Pretzer, W. *et al, J. Am. Chem. Soc.*, 1973, **95**, 931 (*ms*)
Pretzer, W. *et al, Inorg. Chem.*, 1974, **13**, 2779 (*nmr*)
Pretzer, W. *et al, J. Am. Chem. Soc.*, 1976, **98**, 1441 (*synth, pmr, uv*)

B_9H_9SSe

7-Thia-9-selenaundecaborane(9), 10Cl IC-001187
[72207-44-4]

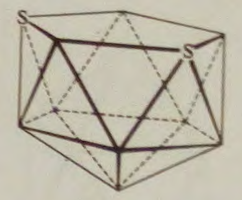


M 217.3
nido-. Colourless solid. Sol. hexane, MeOH, Me_2CO. Mp 313-315°.

Friesen, G.D., *Inorg. Chem.*, 1980, **19**, 458 (*synth, ir, B-11 nmr, ms*)

$B_9H_9S_2$

7,9-Dithiaundecaborane(9), 10Cl IC-001188
[72207-43-3]

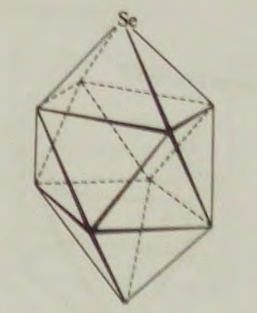


M 170.5
nido-. Colourless solid. Sol. hexane, CH_2Cl_2. Mp 275-276° dec. Purif. from $SSeB_9H_9$ by prep. glc.

Friesen, G.D., *Inorg. Chem.*, 1980, **19**, 458 (*synth, ir, B-11 nmr, ms*)

B_9H_9Se

1-Selenadecaborane(9), 10Cl IC-001189
[72985-72-9]

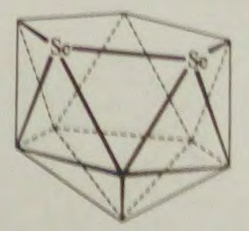


M 185.3
closo-. Colourless cryst. Sol. hexane, CH_2Cl_2. Mp 260-261.5°.

Friesen, G.D. *et al, Inorg. Chem.*, 1980, **19**, 1485 (*synth, ir, B-11 nmr, ms*)

$B_9H_9Se_2$

7,8-Diselenaundecaborane(9), 11Cl, 10Cl IC-001190
[67702-69-6]



M 264.2
nido-. Colourless cryst. Sol. hexane, CH_2Cl_2. Mp 340-342°.

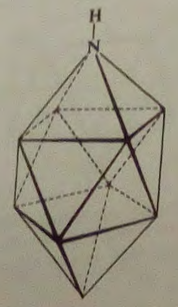
Little, J.L. *et al, Inorg. Chem.*, 1977, **16**, 869 (*synth, ir, B-11 nmr, ms*)
Friesen, G.D., *Inorg. Chem.*, 1980, **19**, 458 (*synth*)
Base, K., *Collect. Czech. Chem. Commun.*, 1983, **48**, 2593 (*synth, ir, pmr, B-11 nmr*)

IC-001191

$B_9H_{10}N$

1-Azadecaborane(10)

[103904-41-2]



M 121.3

closo-. Cryst. (by subl.). Sol. $CHCl_3$. Mp 155-157°.

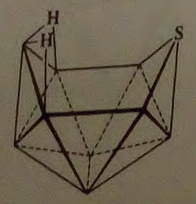
Arafat, A. *et al, Inorg. Chem.*, 1986, **25**, 3757 (*synth, pmr, B-11 nmr, ms, ir*)

IC-001192

$B_9H_{11}S$

6-Thiadecaborane(11), 10CI

[12447-77-7]



M 140.4

nido-. Transparent cryst. Sol. C_6H_6. Mp 76.5°. $Subl._{0.1}$ 70-90°.

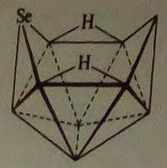
Pretzer, W. *et al, J. Am. Chem. Soc.*, 1976, **98**, 1441 (*synth, struct, nmr*)

IC-001193

$B_9H_{11}Se$

6-Selenadecaborane(11), 11CI, 10CI

[72985-65-0]



M 187.3

nido-. Pale yellow hygroscopic solid. Sol. C_6H_6. Mp 84-85°.

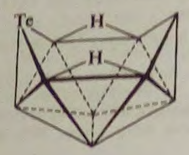
Friesen, G.D. *et al, Inorg. Chem.*, 1980, **19**, 1485 (*synth, B-11 nmr, ms*)

IC-001194

$B_9H_{11}Te$

6-Telluradecaborane(11)

[72985-66-1]



M 235.9

nido-. Pure compd. not isol. Sol. C_6H_6.

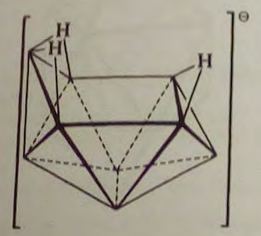
Friesen, G.D. *et al, Inorg. Chem.*, 1980, **19**, 1485 (*synth, B-11 nmr*)

IC-001195

$B_9H_{12}^{\ominus}$

Dodecahydrononaborate(1−), 11CI, 10CI, 9CI, 8CI

[12430-26-1]



M 109.3 (ion)

nido-.

Me_4N salt: [67537-67-1].
Colourless cryst.

Et_4N salt: [51464-40-5].
Colourless cryst. Sol. CH_2Cl_2.

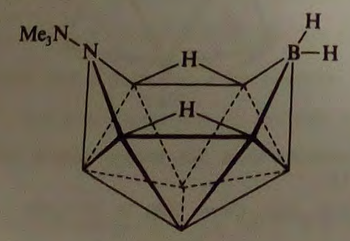
Graybill, B.M. *et al, J. Chem. Soc.*, 1961, **83**, 2669 (*synth*)
Siedle, A.R. *et al, Inorg. Chem.*, 1974, **13**, 1756 (*synth, B-11 nmr*)
Bould, J. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2477 (*pmr, B-11 nmr*)

IC-001196

$B_9H_{12}N$

6-Azadecaborane(12), 11CI, 9CI, 8CI

[58985-53-8]



Me_3N complex

M 123.4

nido-. Synth. by degradation of $NaB_{10}H_{12}NO_2$ by conc. H_2SO_4 or from $NaB_9H_{12}NH$ + conc. H_2SO_4 in pentane. Air sensitive colourless cryst. Sol. CH_2Cl_2, CCl_4, MeCN. Subl. 79-80°.

Me_3N complex: [11092-85-6].
Synth. from $[Me_4N]Me_2NNB_9H_{12}$ and MeI in MeCN. Colourless cryst. (MeCN/EtOH). Dec. at 176.5° without melting.

MeCN complex:
$C_2H_{15}B_9N_2$ M 164.4

Synth. by oxidation of $[B_9H_{12}NH]^{\ominus}$ with Br_2 in MeCN. Slowly dec. in air. Mp 85-88°.

Cyclohexylisocyanide complex: [103904-39-8].
$C_7H_{23}B_9N_2$ M 232.5
Colourless cryst. (MeCl/hexane). Sol. CH_2Cl_2. Mp 115-117°. Cyclohexylisocyanide at 6-position.

Py complex: [103904-40-1].
Synth. from fresh $B_9H_{11}NH$ and Py in pentane. Yellow plates (MeCl/hexane). Mp 122-123°.

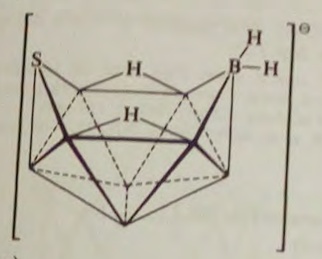
Hertler, W.R. *et al, Inorg. Chem.*, 1967, **6**, 1696 (*synth*)
Base, K. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 1162 (*synth, ir, pmr, B-11 nmr, uv, ms*)
Arafat, A. *et al, Inorg. Chem.*, 1986, **25**, 3757 (*synth, cryst struct, B-11 nmr*)
Kester, J.G. *et al, Inorg. Chem.*, 1988, **27**, 4529 (*synth, B-11 nmr, ms*)

IC-001197

$B_9H_{12}S^{\ominus}$

Dodecahydro-6-thiadecaborate(1−), 11CI, 10CI, 9CI, 8CI

[39448-31-2]



M 141.4 (ion)

arachno-.

Cs salt: [11092-86-7].
Colourless cryst (H_2O). Sol. MeCN.

Me_4N salt: [51293-01-7].
Colourless cryst. (Me_2CO). Sol. MeCN.

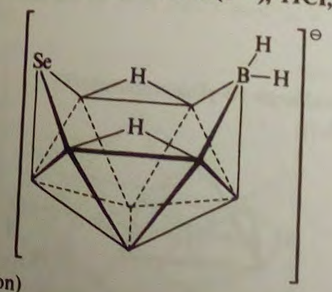
[45979-10-0]

Hertler, W.R. *et al, Inorg. Chem.*, 1967, **6**, 1696 (*synth, ir, B-11 nmr, uv, electrochem*)
Inorg. Synth., 1983, **22**, 226 (*synth, ir, B-11 nmr*)

IC-001198

$B_9H_{12}Se^{\ominus}$

Dodecahydro-6-selenadecaborate(1−), 11CI, 10CI



M 188.3 (ion)

arachno-.

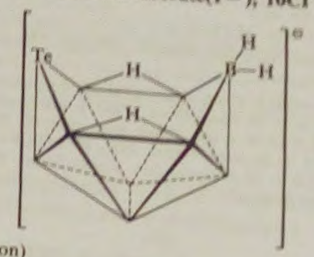
Me_4N salt: [73116-65-1].
Colourless cryst. (MeCN aq.). Sol. Me_2CO, MeCN.
Dec. at 335-340° without melting.

Friesen, G.D. *et al, Inorg. Chem.*, 1980, **19**, 1485 (*synth, ir, B-11 nmr*)

IC-001199

$B_9H_{12}Te^{\ominus}$

Dodecahydro-6-telluradecaborate(1−), 10CI



M 236.9 (ion)

arachno-.

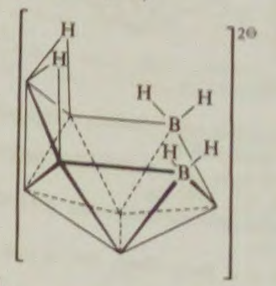
Me_4N salt: [73116-66-2].
Pale yellow cryst. (Me_2CO/MeOH); has limited stability in air. Sol. MeCN.

Friesen, G.D. *et al, Inorg. Chem.*, 1980, **19**, 1485 (*synth, ir, B-11 nmr*)

IC-001200

$B_9H_{13}^{2\ominus}$

Tridecahydrononaborate(2−)



M 110.4 (ion)

arachno-.

Di-Na salt: [119391-53-6].
$B_9H_{13}Na_2$ M 156.3
White solid. Mod. sol. THF.
▷ Some preparations of this salt lead to explosions.

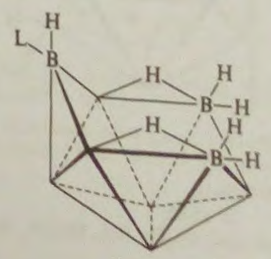
Bis-K[crypt] salt: [119391-52-5].
Colourless cryst. (MeCN/Et_2O). Sol. MeCN.

Getman, T.D. *et al, Inorg. Chem.*, 1989, **28**, 1507 (*synth, ir, pmr, B-11 nmr, cryst struct*)

IC-001201

B_9H_{13}

Nonaborane(13)



L = MeCN

MeCN complex

M 110.4

Obt. as complexes which have *arachno*-structs.

4-MeCN complex: [32357-05-4]. *4-(Acetonitrile) nonaborane(13), 11Cl. Nonaborane(13) compd. with acetonitrile, 8Cl*

$C_2H_{16}B_9N$ M 151.4

Colourless cryst. Sol. MeCN, CH_2Cl_2. Mp > 300°.

arachno-.

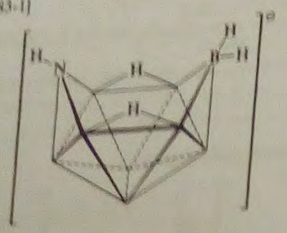
Wang, F.E. *et al, J. Chem. Phys.*, 1961, **35**, 1335 (*cryst struct*)
Graybill, B.M. *et al, Inorg. Chem.*, 1962, **1**, 626 (*synth*)
Benjamin, L.E. *et al, J. Am. Chem. Soc.*, 1963, **85**, 2674 (*synth*)
Bodner, B.M. *et al, Inorg. Chem.*, 1971, **10**, 942 (*B-11 nmr*)
Jacobsen, G.B. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 415 (*synth, B-11 nmr*)

IC-001202

$B_9H_{13}N^{\ominus}$

Tridecahydro-6-azadecaborate(1−), 11Cl, 10Cl, 8Cl

[66272-83-1]



M 124.4 (ion)

arachno-

Cs salt: Colourless cryst. (EtOH/C_6H_6/cyclohexane).

Me_4N salt: [12403-49-5].

Colourless cryst. (aq. AcOH). Sol. MeCN, EtOH. Mp > 300°. Ir ν_{B-H} 3390 cm^{-1}.

Bis(triphenylphosphine)iminium salt: [103885-37-6]. Sol. CH_2Cl_2.

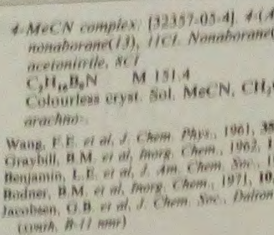
Hertler, W.R. *et al, Inorg. Chem.*, 1987, **6**, 1696 (*synth, pmr, B-11 nmr, ir*)
Base, K. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 1162 (*synth*)
Arafat, A. *et al, Inorg. Chem.*, 1986, **25**, 3757 (*synth, pmr, B-11 nmr, ir*)

IC-001203

$B_9H_{14}^{\ominus}$

Tetradecahydrononaborate(1−), 11Cl, 10Cl, 9Cl, 8Cl

[12430-28-3]



M 111.4 (ion)

arachno-

K salt: [39296-28-1].

$B_9H_{14}K$ M 150.5

Colourless solid (Et_2O). Sol. MeCN, H_2O. Dec. in Et_2O over 24h

Cs salt: [12693-05-0].

B_9CsH_{14} M 244.3

Colourless solid. Insol. C_6H_6.

Me_4N salt: [12545-03-6].

Colourless solid. Insol. C_6H_6.

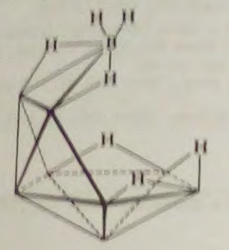
Benjamin, L.E. *et al, J. Am. Chem. Soc.*, 1963, **85**, 2674 (*synth, str*)
Inorg. Synth., 1989, **26**, 1 (*synth, B-11 nmr*)

IC-001204

B_9H_{15}

Nonaborane(15), 10Cl

[19465-30-6]



M 112.4

arachno-. Cryst. solid (pentane at −30°), liq. at r.t. Sol. pentane. Mp 2.5°.

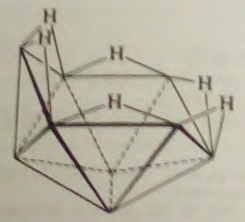
Simpson, P. *et al, J. Chem. Phys.*, 1961, **35**, 1340 (*cryst struct*)
Burg, A. *et al, Inorg. Chem.*, 1962, **1**, 725 (*ir*)
Ditter, J. *et al, Inorg. Chem.*, 1966, **5**, 118 (*ms*)
Schaeffer, R. *et al, Inorg. Chem.*, 1972, **11**, 3102 (*synth, nmr*)

IC-001205

B_9H_{15}

Isononaborane(15), 10Cl

[12447-79-9]



M 112.4

arachno-. Solid, dec. above −30°. Sol. pentane.

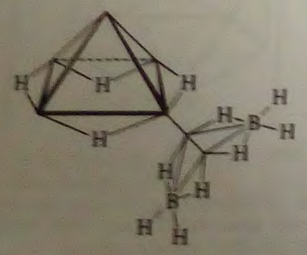
Dobson, J. *et al, Inorg. Chem.*, 1968, **7**, 399 (*synth*)
Moody, D. *et al, Inorg. Chem.*, 1976, **15**, 233 (*nmr*)

IC-001206

B_9H_{17}

2'-(1-Tetraboran-10-yl)pentaborane(9)

[93110-35-1]



M 114.4

conjuncto-. Synth. from B_9H_{11} + B_2H_6 using $PtBr_2$ as catalyst at 25°. Dec. in liquid state above −20°

Swidler, L.G. *et al, J. Am. Chem. Soc.*, 1984, **106**, 7793 (*synth, B-11 nmr, pmr*)

$B_{10}BeH_{20}$

Bis[decahydropentaborato(1−)]beryllium

[65762-38-1]

IC-001207

M 137.2

conjuncto-. The two B_5H_{10} units are staggered. Air- and moisture sensitive volatile solid (1,3-dimethylbenzene at −37°). Sol. C_6H_6, toluene. Mp 52°. Cf. (η^5-2,4-Cyclopentadien-1-yl)[decahydropentaborato(1−)] beryllium, IC-004759.

Pyrophoric, toxic.

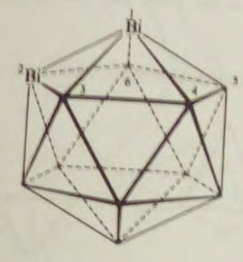
[65859-23-6]

Gaines, D.F. *et al, Inorg. Chem.*, 1978, **17**, 1238, 1242 (*synth, ir, B-11 nmr, pmr, cryst struct*)
Bicerano, J. *et al, Inorg. Chem.*, 1979, **18**, 1565 (*theory*)
Gaines, D.F. *et al, J. Magn. Reson.*, 1981, **44**, 84 (*Be-9 nmr*)

$B_{10}Bi_2H_{10}$

1,2-Dibismadodecaborane(10)

IC-001208



M 536.1

closo-. Colourless cryst. (Me_2CO). Sol. toluene, 1,2-dichloroethane. Mp > 500°. Darkens at > 350°.

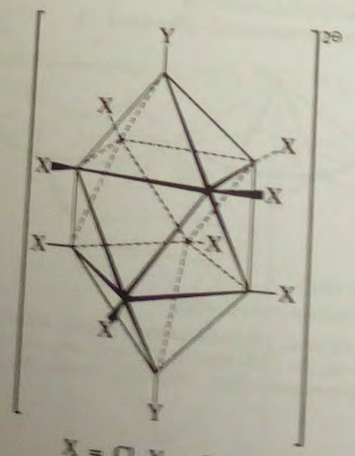
Little, J.L. *et al, Inorg. Chem.*, 1990, **29**, 804 (*synth, ir, B-11 nmr, ms, cryst struct*)

$B_{10}Br_2Cl_8^{2\ominus}$

1,10-Dibromooctachlorodecaborate(2−), 10Cl, 9Cl, 8Cl

IC-001209

[61674-46-2]



X = Cl, Y = Br

M 551.5 (ion)

closo-.

Di-Cs salt: [12447-81-3].

Colourless cryst. + $1H_2O$ (H_2O). Sol. H_2O, MeCN.

Bis-Me_4N salt: Colourless cryst. (aq. EtOH). Sol. MeCN. Darkens at 340° - does not melt below 400°.

Knoth, W.H. *et al, J. Am. Chem. Soc.*, 1967, **89**, 4842 (*synth, str, ir*)

$B_{10}Br_{10}^{2\ominus}$

Decabromodecaborate(2−), 11Cl, 10Cl, 9Cl, 8Cl

IC-001210

As 1,10-Dibromooctachlorodecaborate(2−), IC-001209 with

X = Y = Br

M 907.1 (ion)

closo-.

Di-Cs salt: [12356-10-4].

$B_{10}Br_{10}Cs_2$ M 1172.9

Colourless cryst. (H_2O). Sol. H_2O. V. stable to heat and chemical attack.

Bis-Me_4N salt: Colourless cryst. (H_2O). Sol. H_2O, MeCN. V. stable to chemical attack.

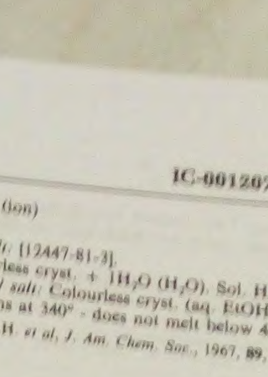
Muetterties, E.L. *et al, J. Am. Chem. Soc.*, 1962, **84**, 2506 (*raman*)
Knoth, W.H. *et al, Inorg. Chem.*, 1964, **3**, 159 (*synth, str, ir, B-11 nmr, electrochem*)
Klanberg, F. *et al, Inorg. Chem.*, 1966, **5**, 1955 (*synth*)
Fr. Pat., 1 496 704, (1968); *CA*, 1968, **69**, 20836 (*synth, use*)

$B_{10}Br_{10}$

Decabromodecaborane(10), 11Cl

IC-001211

[84879-93-6]



X = Y = Br

M 907.1

Coloured (?) solid. Sol. pentane, CH_2Cl_2, CCl_4, BBr_3. Stable below 200° *in vacuo*.

Reason, M.S. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 1789 (*synth*)
Kutz, N.A. *et al, Inorg. Chem.*, 1980, **19**, 3295 (*synth, ms, B-11 nmr*)

$B_{10}Ca_2H_{14}O_{28}$

Priceite, 10Cl

IC-001212

Pandermite

[12409-13-7]

$Ca_2[B_5O_6(OH)_3].H_2O$ or $Ca_4B_{10}O_{14}(OH)_{12}.5H_2O$

M 698.5

$B_{10}Cl_2CuH_{12}^{2\ominus}$ – $B_{10}FeH_{10}^{\ominus}$

Struct. unknown. Two common formulations given.
Borate mineral. Colourless solid. Spar. sol. H_2O.

[61383-61-7]

Christ, C.L., *J. Geol. Educ.*, 1972, **20**, 235 (*rev*)
Ross, S.D., *Infrared Spectra of Minerals*, London, 1974, 205 (*ir*)
Bowden, G.H. *et al*, *Mellor Compr. Treat. Inorg. Theor. Chem.*, Longman, London, 1980, V/A, 555.
Fukushige, Y. *et al*, *C-A*, 1982, **97**, 119443 (*synth*)

IC-001213

$B_{10}Cl_2CuH_{12}^{2\ominus}$

Dichloro[tridecahydrodecaborato(1−)]cuprate(2−), 8CI

[12555-75-8]

$[Cl_2CuB_{10}H_{13}]^{2\ominus}$

M 255.6 (ion)
Struct. prob. based on $[B_{10}H_{13}]^{\ominus}$. Synth. from $CuCl_2.2H_2O$ in THF + decaborane and NaH in Et_2O at −10°.
Bis-Et_4N salt: Bright yellow solid (THF). Darkens at 145°, does not melt below 400°.

Muetterties, E.L. *et al*, *Inorg. Chem.*, 1970, **9**, 2447 (*synth, P-31 nmr, B-11 nmr*)

IC-001214

$B_{10}Cl_8N_2^{2\ominus}$

1,10-Diazidooctachlorodecaborate(2−), 8CI

As 1,10-Dibromooctachlorodecaborate(2−), IC-001209 with

X = Cl, Y = N_3

M 475.7 (ion)
closo-.
Di-Cs salt: Colourless cryst. (H_2O). Sol. H_2O, MeCN.
▷ Shock sensitive; explodes on heating to 224°.

Knoth, W.H. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 115 (*synth*)
Knoth, W.H., *J. Am. Chem. Soc.*, 1966, **88**, 935 (*synth, uv, ir*)

IC-001215

$B_{10}Cl_{10}^{2\ominus}$

Decachlorodecaborate(2−), 11CI, 10CI, 9CI, 8CI

[51358-33-9]

As 1,10-Dibromooctachlorodecaborate(2−), IC-001209 with

X = Y = Cl

M 462.6 (ion)
closo-.
Di-Cs salt: [12360-16-6].
$B_{10}Cl_{10}Cs_2$ M 728.4
Colourless cryst. (H_2O). Sol. H_2O. Stable in air up to 400°
Di-H_3O compd.: Decachlorodecaboric acid
$B_{10}Cl_{10}H_6O_2$ M 500.6
Colourless solid + $2H_2O$. Sol. H_2O, MeCN; insol. C_6H_6, CCl_4. Strong acid, comparable with H_2SO_4.
Bis-Me_4N salt: [80860-73-7].
Colourless cryst. (aq. EtOH). Sol. MeCN.

Muetterties, E.L. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 2506 (*raman*)
Forstner, J.A. *et al*, *Inorg. Chem.*, 1964, **3**, 155 (*synth, ir*)
Knoth, W.H. *et al*, *Inorg. Chem.*, 1964, **3**, 159 (*synth, uv, ir, B-11 nmr, electrochem*)
Curtis, Z.B. *et al*, *Inorg. Chem.*, 1974, **13**, 1760 (*synth, ir*)
Saulys, D.A. *et al*, *Inorg. Chem.*, 1983, **22**, 1821 (*synth*)

IC-001216

$B_{10}Cl_{10}$

Decachlorodecaborane(10), 11CI, 10CI

[61674-49-3]

As Decabromodecaborane(10), IC-001211 with

X = Y = Cl

M 462.6
Air and moisture sensitive orange-brown cryst. Stable to 350° *in vacuo*.

Reason, M.S. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 1789 (*synth, ms*)
Awad, S.B. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 395 (*synth, ms*)
Saulys, D.A. *et al*, *Inorg. Chem.*, 1983, **22**, 1821 (*synth, ms, B-11 nmr*)

IC-001217

$B_{10}EuH_{10}$

Europium(*II*) decahydrodecaborate

[123623-29-0]

$EuB_{10}H_{10}$

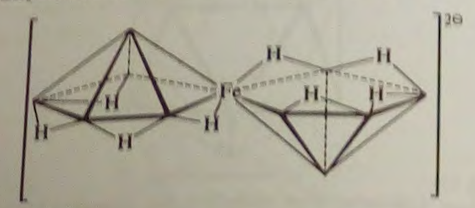
M 270.1
Believed to be essentially ionic: $Eu^{2\oplus}B_{10}H_{10}^{2\ominus}$. Grey-green solid. Sol. Py → bright yellow soln. Yb analogue also isol.

White, J.P. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 8946 (*synth, ir*)

IC-001218

$B_{10}FeH_{18}^{2\ominus}$

Bis[nonahydropentaborato(2−)]ferrate(2−)



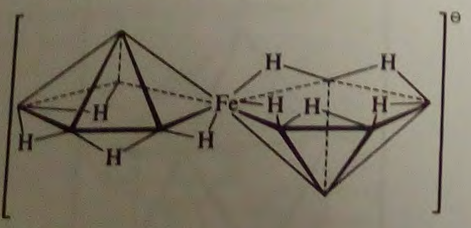
M 182.0 (ion)
Di-K salt: Rust red solid.

Shore, S.G. *et al*, *Abstr. 4th Internat. Meeting Boron Chemistry*, Imeboron IV, 1979 Abstract 07 (*synth*)
Compr. Organomet. Chem., Pergamon, Oxford, 1982, **6**, 879 (*synth*)

IC-001219

$B_{10}FeH_{19}^{\ominus}$

[Decahydropentaborato(1−)] [nonahydropentaborato(2−)]ferrate(1−)



M 183.1 (ion)
K salt: Yellow-brown solid.

Shore, S.G. *et al*, *Abstr. 4th Internat. Meeting Boron Chemistry*, Imeboron IV, 1979 Abstract 07 (*synth, pmr, B-11 nmr*)
Compr. Organomet. Chem., Pergamon, Oxford, 1982, **6**, 879 (*synth*)

$B_{10}FeH_{20}$

Bis[decahydropentaborato(1−)]iron

IC-001220

M 184.1
Dark brown solid.

Shore, S.G. *et al*, *Abstr. 4th Internat. Meeting Boron Chemistry*, Imeboron IV, 1979 Abstract 07 (*synth, proposed struct*)
Compr. Organomet. Chem., Pergamon, Oxford, 1982, **6**, 879 (*synth*)

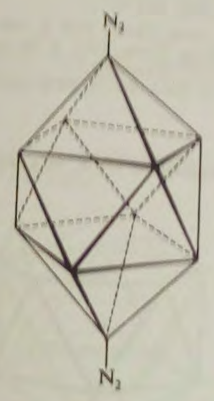
$B_{10}H_8N_4$

1,10-Bis(diazo)decaborane(10)

1,10-Bis(dinitrogen)decaborane(10), 11CI. Decaborane(8) compd. with nitrogen (1:2), 8CI

IC-001221

[12008-54-7]



M 172.2
closo-. Colourless cryst. (50% aq. EtOH). Sol. C_6H_6, MeCN, CH_2Cl_2; reacts with C_6H_6.

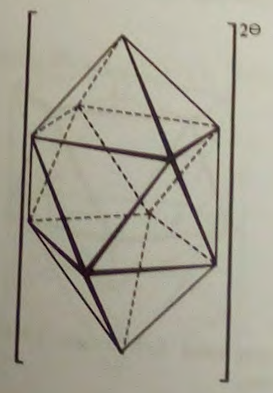
Knoth, W.H., *J. Am. Chem. Soc.*, 1966, **88**, 935 (*synth, uv, ir, B-11 nmr*)
Whelan, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 2469 (*pe, ms, cryst struct*)
Knoth, W.H., *Organometallics*, 1985, **4**, 207 (*synth, reactions*)

$B_{10}H_{10}^{2\ominus}$

Decahydrodecaborate(2−), 11CI, 10CI, 9CI, 8CI

IC-001222

[12356-12-6]



M 118.1 (ion)
closo-. Salts are remarkably stable to chemical attack.
Di-Cs salt: [12008-58-1]
$B_{10}Cs_2H_{10}$ M 384.6
Colourless cryst. (H_2O). Sol. MeCN, H_2O. Stable to ≈655° (sealed tube).
Di-H_3O compd.: Decahydrodecaboric acid
$B_{10}H_{16}O_2$ M 156.2
Colourless cryst. + $2H_2O$ (H_2O). Sol. H_2O, MeCN. Mp 202-206° dec. Stronger acid than H_2SO_4.
Bis-Et_3NH salt: Colourless cryst. (aq. EtOH). Sol. H_2O, MeCN. Mp 230-232°.

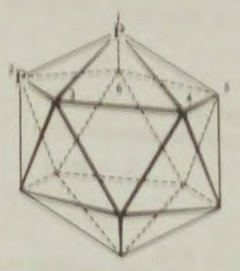
Knoth, W.H. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 1056 (*synth, B-11 nmr*)
Dobrott, R.D. *et al*, *J. Chem. Phys.*, 1962, **37**, 1977 (*cryst struct*)
Muetterties, E.L. *et al*, *Inorg. Chem.*, 1964, **3**, 444 (*synth, uv, ir, B-11 nmr*)
Inorg. Synth., 1967, **9**, 16 (*synth, ir*)
Hall, J.H. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 770 (*ir*)

$B_{10}H_{10}P_2$

1,2-Diphosphadodecaborane(10), 12CI

IC-001223

[119593-19-0]



M 180.1
closo-. Colourless solid with sweet odour. Sol. THF, $CHCl_3$, hexane. Mp 397-399°.

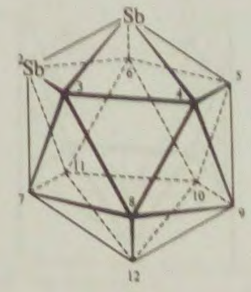
Little, J.L. *et al*, *Inorg. Chem.*, 1989, **28**, 1087 (*synth, ir, pmr, B-11 nmr, P-31 nmr, ms*)

$B_{10}H_{10}Sb_2$

1,2-Distibadodecaborane(10), 10CI

IC-001224

[69531-87-9]



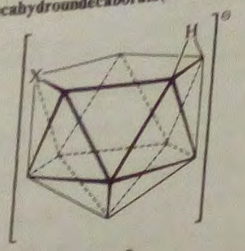
M 361.6
closo-. Off-white solid. Sol. C_6H_6, DMF. Mp >400° dec.

Little, J.L., *Inorg. Chem.*, 1979, **18**, 1598 (*synth, ir, B-11 nmr, ms*)

IC-001225

$B_{10}H_{11}S^{\ominus}$

7-Thiaundecahydroundecaborate(1 –), 10CI, 9CI, 8CI



X = S

M 151.2 (ion)
nido-.
Cs salt: [12421-67-9].
$B_{10}CsH_{11}S$ M 284.1
Colourless cryst. (H_2O).
Me_4N salt: [52656-11-8].
Colourless cryst. ($MeCN/C_6H_6$).

Hertler, W.R. *et al, Inorg. Chem.*, 1967, **6**, 1696 (*synth, ir, B-11 nmr, uv*)

IC-001226

$B_{10}H_{11}Se^{\ominus}$

7-Selenaundecahydroundecaborate(1 –), 10CI

As 7-Thiaundecahydroundecaborate(1 –), IC-001225 with

X = Se

M 198.1 (ion)
nido-.
Me_4N salt: [61702-39-4].
Colourless cryst. (Me_2CO); unstable in air after few days. Sol. MeCN, CH_2Cl_2.
Et_4N salt: Colourless cryst. (CH_2Cl_2).

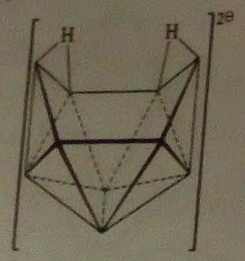
Little, J.L. *et al, Inorg. Chem.*, 1977, **16**, 869 (*synth, ir, B-11 nmr*)
Reed, D. *et al, Polyhedron*, 1988, **7**, 17 (*synth, pmr, B-11 nmr, cryst struct*)

IC-001227

$B_{10}H_{12}^{2\ominus}$

Dodecahydrododecaborate(2 –), 10CI, 9CI, 8CI

[12430-37-4]



M 120.2 (ion)
nido-.
Di-Na salt: [12046-70-7].
$B_{10}H_{12}Na_2$ M 166.1
Colourless solid; hygroscopic, dec. in moist air. Insol. Et_2O.
Bis-Me_4N salt: Colourless solid.

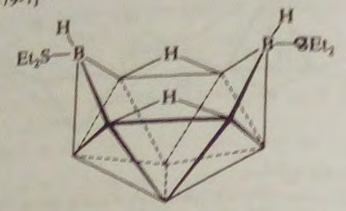
Wilkes, P.H. *et al, J. Am. Chem. Soc.*, 1966, **88**, 3441 (*synth, ir*)
Greenwood, N.N. *et al, J. Chem. Soc. A*, 1969, 2334 (*synth, ir, uv*)

IC-001228

$B_{10}H_{12}$

Decaborane(12)

[32124-79-1]



Bis-Et_2S complex

M 120.2
Isol. as complex with Et_2S.
Bis-Et_2S complex: [32174-79-1]. *Decaborane(12) compd. with 1,1'-thiobis[ethane] (1:2), 10CI*
$C_8H_{32}B_{10}S_2$ M 300.5
Important precursor to 1,2-dicarbadodecaborane(12) derivs. White solid. Mp 91°.

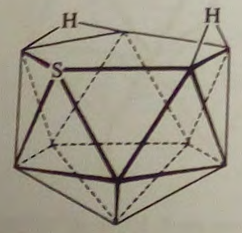
Heyling, T.L. *et al, Inorg. Chem.*, 1963, **2**, 1089 (*synth*)
Hyatt, D.E. *et al, Inorg. Chem.*, 1967, **6**, 630 (*nmr*)
Inorg. Synth., 1967, **10**, 95 (*synth*)
Cragg, R.H. *et al, J. Chem. Soc. A*, 1970, 1817 (*uv*)

IC-001229

$B_{10}H_{12}S$

7-Thiaundecaborane(12), 10CI, 9CI, 8CI

[12421-68-0]



M 152.2
nido-. Colourless solid. Sol. MeCN, C_6H_6; spar. sol. H_2O.

[58984-44-4, 60294-96-4]

Hertler, W.R. *et al, Inorg. Chem.*, 1967, **6**, 1696 (*synth, ir, B-11 nmr, uv*)
Kang, S.O. *et al, Inorg. Chem.*, 1988, **27**, 3298 (*synth*)

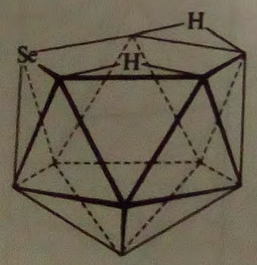
IC-001230

$B_{10}H_{12}Se$

7-Selenaundecaborane(12), 10CI

7-Selenoundecaborane(12)

[61649-90-9]



M 199.1
nido. Colourless solid. Sol. hexane, $CHCl_3$, MeCN. Mp 239-241° dec.

[67702-68-5]

Little, J.L. *et al, Inorg. Chem.*, 1977, **16**, 869 (*synth, ir, B-11 nmr, ms*)
Wright, W.F. *et al, J. Magn. Reson.*, 1978, **30**, 595 (*B-11 nmr*)

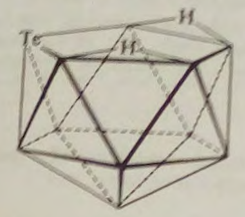
IC-001231

$B_{10}H_{12}Te$

7-Telluraundecaborane(12), 10CI

7-Telluroundecaborane(12)

[61649-91-0]



M 247.8
nido-. Colourless solid. Sol. hexane, $CHCl_3$. Mp 244-246° dec.

[67702-69-6]

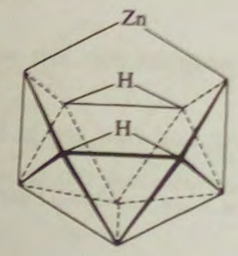
Little, J.L. *et al, Inorg. Chem.*, 1977, **16**, 869 (*synth, ir, B-11 nmr*)
Wright, W.F. *et al, J. Magn. Reson.*, 1978, **30**, 595 (*B-11 nmr*)

IC-001232

$B_{10}H_{12}Zn$

[η^4-Dodecahydrodecaborato(2 –)]zinc

Decaborane(14)-6,9-diylzinc



M 185.5
Proposed struct.
Et_2O complex: [19287-44-6].
Air-sensitive yellow cryst. (CH_2Cl_2/Et_2O). Sol. H_2O, EtOH, MeCN, CH_2Cl_2, $ClCH_2CH_2Cl$. Loses Et_2O at 130°.
THF complex: [19154-51-9].
Air-sensitive yellow cryst.

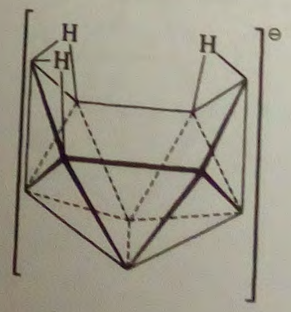
Greenwood, N.N. *et al, J. Chem. Soc. A*, 1968, 15 (*synth, uv, ir, pmr, B-11 nmr*)

IC-001233

$B_{10}H_{13}^{\ominus}$

Tridecahydrodecaborate(1 –), 11CI, 10CI, 9CI, 8CI

[12430-38-5]



M 121.2 (ion)
nido-.
Na salt: [32200-63-8].
$B_{10}H_{12}Na$ M 144.2
Pale yellow solid. Sol. ethers.
Me_4N salt: Colourless solid. Sol. ethers.

[12008-65-0, 36972-59-6]

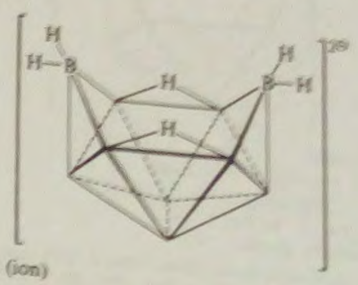
Miller, J.J. *et al, J. Am. Chem. Soc.*, 1959, **81**, 4501 (*synth, ir, uv*)
Blay, N.J. *et al, J. Chem. Soc.*, 1962, 3416 (*synth, ir, uv, B-11 nmr*)
Greenwood, N.N. *et al, J. Chem. Soc. A*, 1969, 2334 (*synth, ir, uv*)
Siedle, A.R. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 3671 (*B-11 nmr*)

IC-001234

$B_{10}H_{14}^{2\ominus}$

Tetradecahydrodecaborate(2 –), 9CI, 8CI

[12430-39-6]



M 122.2 (ion)
arachno-.
Di-Cs salt:
$B_{10}Cs_2H_{14}$ M 388.0
Colourless cryst. (H_2O).
Bis-Me_4N salt: [37209-64-6].
Colourless cryst.

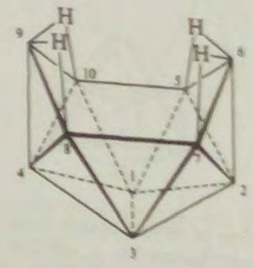
Muetterties, E.L. *et al, Inorg. Chem.*, 1963, **2**, 647 (*synth, ir, B-11 nmr*)
Chambers, J.Q. *et al, J. Am. Chem. Soc.*, 1968, **90**, 6056 (*electrochem*)
Kendall, D.S. *et al, Inorg. Chem.*, 1973, **12**, 546 (*cryst struct*)

IC-001235

$B_{10}H_{14}$

Decaborane(14), 10CI

[17702-41-9]



M 122.2
nido-. Precursor for carboranes. Cryst. solid by subl. Sol. CS_2. Mp 99.6°. Bp 213° (221°).
▷ Toxic. HD1400000.
6-Hydroxy: [98514-25-1]. *6-Hydroxydecaborane(13), 11CI*
Intermed. for production of metallaboranes.
Hygroscopic white cryst. (cyclohexane). Sol. cyclohexane. Dec. >160°.

Stock, A. *et al, Ber.*, 1913, **46**, 3353 (*synth*)
Kasper, J. *et al, Acta Crystallogr.*, 1950, **3**, 436 (*cryst struct*)
Keller, W. *et al, J. Chem. Phys.*, 1952, **20**, 1749 (*uv, ir*)
Quayle, A., *J. Appl. Chem.*, 1959, **9**, 395 (*ms*)
Williams, R., *Inorg. Chem.*, 1965, **4**, 1504 (*nmr*)

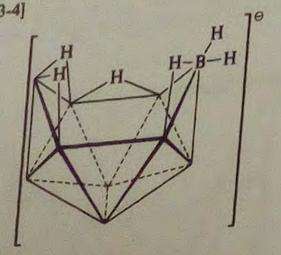
Holzmann, R. *et al*, *Production of the Boranes and Related Research*, Academic Press, New York, 1967, 102 (*synth*)
Bodner, G. *et al*, *Inorg. Chem.*, 1970, **9**, 1421 (*nmr*)
Toft, M. *et al*, *Inorg. Chem.*, 1982, **21**, 1952 (*synth*)
Greenwood, N.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 953 (*deriv, synth, ir, ms, B-11 nmr, pmr*)

IC-001236

$B_{10}H_{15}^{\ominus}$

Pentadecahydrodecaborate(1−), 11CI, 9CI, 8CI

[39448-33-4]



M 123.2 (ion)
arachno-; possible struct. shown.
Na salt: [12008-67-2].
$B_{10}H_{15}Na$ M 146.2
Sol. MeCN, glyme.

Schaeffer, R.O. *et al*, *Inorg. Chem.*, 1964, **3**, 1638 (*synth, B-11 nmr*)
Rupp, E.B. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 5562 (*synth, electrochem*)
Rietz, R.R. *et al*, *Inorg. Chem.*, 1973, **12**, 2100 (*pmr, B-11 nmr*)

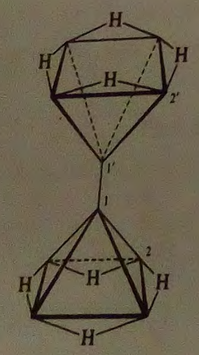
IC-001237

$B_{10}H_{16}$

1,1′-Bipentaborane(9), 10CI

1-(1-Pentaboran(9)yl)pentaborane(9). Decaborane(16)

[71595-75-0]



M 124.2
Linked *nido-*. One of three isomeric decaborane(16)'s. See also 1,2′-Bipentaborane(9), IC-001238 and 2,2′-Bipentaborane(9), IC-001239. Solid, stable at 25°. Mp 81°. Sublimes.

Grimes, R. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1962, **48**, 496 (*synth, ir*)
Ardini, L. *et al*, *Inorg. Chem.*, 1973, **12**, 798 (*synth*)

$B_{10}H_{16}$ IC-001238

1,2′-Bipentaborane(9), 10CI

1-(2-Pentaboran(9)yl)pentaborane(9). Decaborane(16)

[31831-99-9]

M 124.2
Linked *nido*. Solid or liq. Mp 18.4°.

Gaines, D. *et al*, *Inorg. Chem.*, 1971, **10**, 1096 (*nmr, ir, ms*)
Gaines, D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 380 (*synth*)
Heppert, J.A. *et al*, *Inorg. Chem.*, 1984, **23**, 14.

IC-001239

$B_{10}H_{16}$

2,2′-Bipentaborane(9), 10CI

2-(2-Pentaboran(9)yl)pentaborane(9). Decaborane(16)

[28775-81-7]

M 124.2
Linked *nido*. Liq. Mp −20.5° (−22.8°).

Gaines, D. *et al*, *Inorg. Chem.*, 1971, **10**, 1096 (*nmr, ir, ms*)
Rietz, R. *et al*, *Inorg. Chem.*, 1972, **11**, 1242 (*nmr*)
Gaines, D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 380 (*synth*)
Heppert, J.A. *et al*, *Inorg. Chem.*, 1984, **23**, 14.

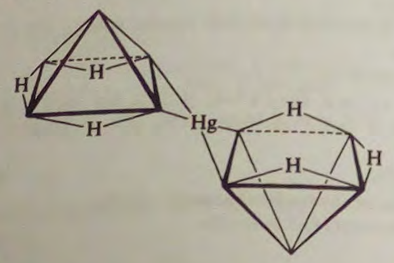
IC-001240

$B_{10}H_{16}Hg$

Bis[(2,3-η)-octahydropentaborato(1−)]mercury, 10CI

Bis(pentaboran(9)-2-yl)mercury, 10CI

[70850-80-5]



M 324.8
Mod. air-stable sublimable cryst. Spar. sol. org. solvs. Mp 161-162°.

[73608-25-0]

Hosmane, N.S. *et al*, *Inorg. Chem.*, 1979, **18**, 2886 (*synth, ir, pmr, B-11 nmr, ms*)
Nelson, M.A. *et al*, *Inorg. Chem.*, 1981, **20**, 3579 (*synth, B-11 nmr*)
Venable, T.L. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 29 (*B-11 nmr*)

$B_{10}I_{10}^{2\ominus}$ IC-001241

Decaiododecaborate(2−), 11CI, 8CI

As 1,10-Dibromooctachlorodecaborate(2−), IC-001209 with

X = Y = I

M 1377.1 (ion)
closo-.
Di-Cs salt: [88423-95-4].
Colourless solid + 1CsI (H_2O). Sol. H_2O.
Bis-H_3O compd.: Decaiododecaboric acid
$B_{10}H_6I_{10}O_2$ M 1415.2
Colourless solid + $6H_2O$ (H_2O). Sol. H_2O.

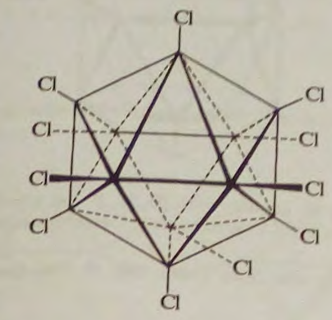
Knoth, W.K., *J. Am. Chem. Soc.*, 1962, **84**, 1056 (*synth*)
Knoth, W.K. *et al*, *Inorg. Chem.*, 1964, **3**, 159 (*synth, ir, electrochem*)

$B_{11}Cl_{11}$ IC-001242

Undecachloroundecaborane(11), 11CI

Boron chloride ($B_{11}Cl_{11}$), 10CI. Undecaboron undecachloride

[12230-26-1]



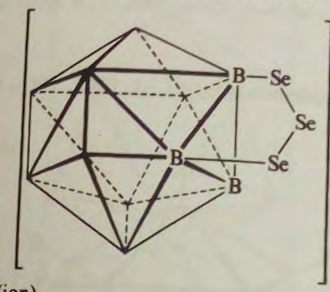
M 508.9
V. sensitive to air and moisture. Dec. at 350° *in vacuo*.

Lanthier, G.F. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 1569 (*synth, ms*)
Awad, S.B. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 395 (*synth, ms*)
Saulys, D.A. *et al*, *Inorg. Chem.*, 1983, **22**, 1821 (*synth, ms, B-11 nmr*)

$B_{11}H_9Se_3^{2\ominus}$ IC-001243

Nonahydro-5,6-(triselena)undecaborate(2−), 10CI

5,6-(Triselena)nonahydroundecaborate(2−)



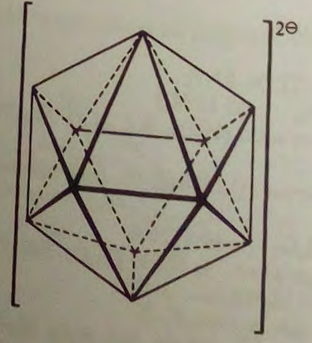
M 364.8 (ion)
closo-B_{11} cage.
Bis-Et_4N salt: [69069-46-1].
Orange plates (aq. MeCN). Cage is fluxional at r.t.

Friesen, G.D. *et al*, *Inorg. Chem.*, 1979, **18**, 755 (*synth, ir, B-11 nmr, uv, cryst struct*)

$B_{11}H_{11}^{2\ominus}$ IC-001244

Undecahydroundecaborate(2−), 11CI, 10CI, 9CI, 8CI

[12430-44-3]



M 130.0 (ion)

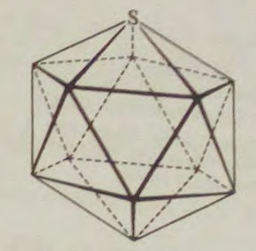
closo-.
Di-Cs salt:
$B_{11}Cs_2H_{11}$ M 395.8
Colourless cryst. (hot H_2O). Sol. H_2O.
Bis-Et_4N salt: [39333-31-8].
Colourless cryst. (MeCN aq.). Sol. MeCN.

Klanberg, F. *et al*, *Inorg. Chem.*, 1966, **5**, 1955 (*synth, uv, ir, electrochem*)
Inorg. Synth., 1968, **11**, 24 (*synth, uv, ir*)
Tolpin, E.I. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 2384 (*B-11 nmr*)
Muetterties, E.L. *et al*, *Inorg. Chem.*, 1975, **14**, 950 (*B-11 nmr*)

$B_{11}H_{11}S$

1-Thiadodecaborane(11) IC-001245

[56464-75-6]



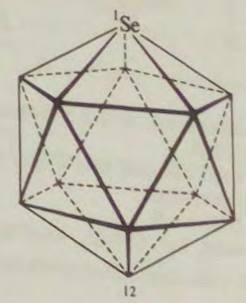
M 162.0
closo-. White cryst. Sol. CS_2, CH_2Cl_2. Mp 325° (sealed tube). Subl. >240°, Subl. >50° *in vacuo*.

Plešek, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 127 (*synth, ms, ir, nmr*)
Pretzer, W. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1441 (*synth, ms, uv, nmr*)

$B_{11}H_{11}Se$

1-Selenadodecaborane(11), 10CI IC-001246

[68027-10-1]



M 208.9
closo-. Colourless cryst. (heptane). Sol. CH_2Cl_2, toluene, $CHCl_3$. Mp 390-395°.
12-Iodo: 12-Iodo-1-selenadodecaborane(11)
$B_{11}H_{10}ISe$ M 334.8
Colourless cryst. (heptane). Sol. CH_2Cl_2, C_6H_6, hexane. Mp 213-215°.

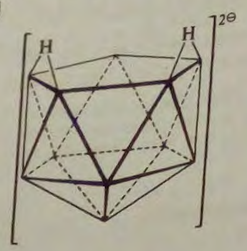
Todd, L.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 349 (*synth, ir, B-11 nmr*)
Ferguson, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 699 (*cryst struct*)
Ni Dhuthghaill, O. *et al*, *Proc. R. Ir. Acad., Sect. B*, 1989, **89**, 461 (*pe, deriv, synth, ir, B-11 nmr, ms, cryst struct*)

IC-001247

$B_{11}H_{13}^{2\ominus}$

Tridecahydroundecaborate(2−), 11CI, 10CI, 9CI, 8CI

[12448-04-3]



M 132.0 (ion)
nido-.
Di-Cs salt:
$B_{11}Cs_2H_{13}$ M 397.8
V. faint yellow cryst. (aq. CsOH).
Bis-Me_4N salt: Colourless cryst. (H_2O).

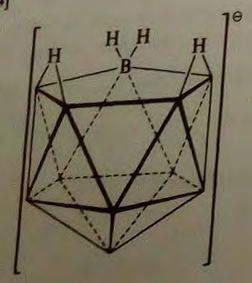
Aftandilian, V.D. *et al, Inorg. Chem.*, 1962, **1**, 734 (*synth, ir*)
Frischie, C.J., *Inorg. Chem.*, 1967, **6**, 1199 (*cryst struct*)
Inorg. Synth., 1968, **11**, 25 (*synth*)

IC-001248

$B_{11}H_{14}^{\ominus}$

Tetradecahydroundecaborate(1−), 11CI, 10CI, 9CI, 8CI

[12448-05-4]



M 133.0 (ion)
nido-.
Na salt: Colourless cryst. + 2.5-3 dioxan (glyme).
Cs salt: [12008-72-9].
Pale yellow solid (dioxan/THF). Sol. 1,2-dimethoxyethane, H_2O.
Et_3NH salt: [12106-44-4].
Pale yellow solid. Sol. CH_2Cl_2, MeOH; insol. H_2O.

Aftandilian, V.D. *et al, Inorg. Chem.*, 1962, **1**, 734 (*synth, ir, pmr, B-11 nmr, uv*)
Inorg. Synth., 1967, **10**, 81 (*synth, ir*)
Dunks, G.B. *et al, Inorg. Chem.*, 1981, **20**, 1692 (*synth*)
Hosmane, N.S. *et al, Inorg. Chem.*, 1987, **26**, 3638 (*synth, B-11 nmr*)
Getman, T.D. *et al, Inorg. Chem.*, 1988, **27**, 2398 (*cryst struct*)

IC-001249

$B_{11}H_{15}$

Undecaborane(15)

M 134.0
*nido-*Struct. by analogy with $[B_{11}H_{14}]^{\ominus}$ but posns. of H atoms on open face unknown. Unstable above 0°. Sol. toluene.

Getman, T.D. *et al, Inorg. Chem.*, 1988, **27**, 2398 (*synth, pmr, B-11 nmr*)

IC-001250

$B_{12}Br_6H_6^{2\ominus}$

Hexabromohexahydrododecaborate(2−), 8CI

$[B_{12}Br_6H_6]^{2\ominus}$

M 615.2 (ion)
closo-. Positions of Br and H not detd.
Di-Cs: [12536-80-0].
$B_{12}Br_6Cs_2$ M 874.9
Colourless cryst. + $1H_2O$ (H_2O). Sol. H_2O. Mp 491-492°.

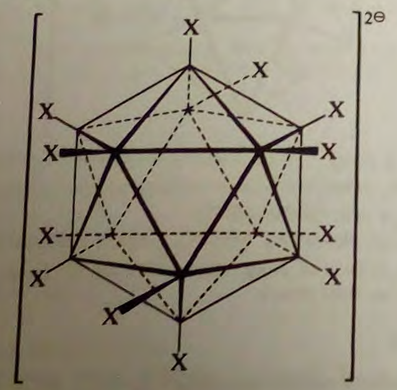
Knoth, W.H. *et al, Inorg. Chem.*, 1964, **3**, 159 (*synth, uv*)

IC-001251

$B_{12}Br_{12}^{2\ominus}$

Dodecabromododecaborate(2−), 11CI, 10CI, 9CI, 8CI

[59271-64-6]



X = Br

M 1088.5 (ion)
closo-.
Di-Cs salt: [12536-87-7].
$B_{12}Br_{12}Cs_2$ M 1354.3
Colourless solid (H_2O). Sol. H_2O, MeCN. Stable to 750°.
Bis-H_3O compd.: [12536-89-9]. *Dodecabromododecaboric acid*
$B_{12}Br_{12}H_6O_2$ M 1126.6
Colourless cryst. + $6H_2O$ (H_2O). Sol. H_2O. Sl. stronger acid than H_2SO_4.
Bis-Me_4N salt: [12546-12-2].
Colourless cryst. (H_2O). Sol. H_2O, MeCN.

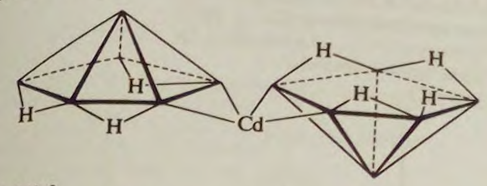
Knoth, W.H. *et al, Inorg. Chem.*, 1964, **3**, 159 (*synth, uv, ir, B-11 nmr, electrochem*)
Kuznetsov, N.T. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1976, **21**, 51 (*synth, ir*)
Kuznetsov, N.T. *et al, Inorg. Materials* (*Engl. Transl.*), 1980, **16**, 958 (*thermal anal*)
Leites, L.A. *et al, Spectrochim. Acta, Part A*, 1982, **38**, 1047 (*ir, raman*)

IC-001252

$B_{12}CdH_{18}$

Bis[(2,3-η)-nonahydrohexaborato(1−)]cadmium, 9CI

[57574-02-4]



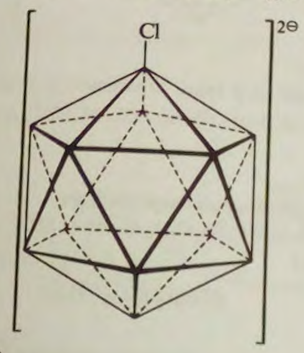
M 260.2
Proposed struct. shown. Synth. from B_6H_{10} and $CdCl_2$ in THF at 6.5°. White photosensitive solid.

Shore, S.G. *et al, Inorg. Chem.*, 1976, **15**, 541 (*synth, pmr, B-11 nmr*)

IC-001253

$B_{12}ClH_{11}^{2\ominus}$

1-Chloroundecahydrododecaborate(2−), 9CI, 8CI



M 176.2 (ion)
closo-.
Di-Cs salt: [89552-26-1].
Colourless cryst. + 1CsCl (H_2O). Sol. H_2O.
Bis-Me_4N salt: [12546-13-3].
Colourless cryst. (H_2O). Sol. H_2O, MeCN.

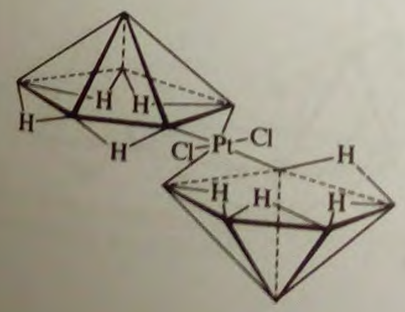
Knoth, W.H. *et al, Inorg. Chem.*, 1964, **3**, 159 (*synth*)
Srebny, H.-G. *et al, Z. Naturforsch., B*, 1984, **39**, 189 (*ir, raman, B-11 nmr*)

IC-001254

$B_{12}Cl_2H_{20}Pt$

Dichlorobis[(4,5-η)-hexaborane(10)]platinum, 9CI

[51177-38-9]



M 415.8
Yellow needles. Sol. toluene. Mp 120° dec. Stable at 25°. Solns. darken unless cooled.

Brennan, J.P. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 354 (*cryst struct*)
Davidson, A. *et al, J. Am. Chem. Soc.*, 1974, **96**, 2802 (*synth, ir, pmr, B-11 nmr*)

IC-001255

$B_{12}Cl_{11}$

Undecachlorododecaborane

Dodecaboron undecachloride. Boron chloride ($B_{12}Cl_{11}$)

$B_{12}Cl_{11}$

M 519.7
Shown to be a mixt. of $B_{10}Cl_{10}$, $B_{11}Cl_{11}$ and $B_{12}Cl_{12}$. Glassy red solid.

Schram, E.P. *et al, Inorg. Chem.*, 1963, **2**, 405 (*synth*)
Lanthier, G.F. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 1569 (*ms*)
Massey, A.G., *Adv. Inorg. Chem. Radiochem.*, 1983, **26**, 1 (*rev*)

IC-001256

$B_{12}Cl_{12}^{2\ominus}$

Dodecachlorododecaborate(2−), 11CI, 10CI, 9CI, 8CI

[39345-60-3]

As Dodecabromododecaborate(2−), IC-001251 with

X = Cl

M 555.1 (ion)
closo-.
Di-Cs salt: [12536-94-6].
$B_{12}Cl_{12}Cs_2$ M 820.9
Colourless cryst. (H_2O). Sol. H_2O. Stable to 700°.
Bis-H_3O salt: [12430-51-2]. *Dodecachlorododecaboric acid*
$B_{12}Cl_{12}H_6O_2$ M 593.2
Colourless solid. Sol. H_2O. Can also be obt. as tetrahydrate.
Bis-tetrahexylammonium salt: Colourless needles (EtOH). Sol. CH_2Cl_2, Me_2CO, MeOH; spar. sol. $CHCl_3$; insol. H_2O,C_6H_6, hexane. Mp 234-235°.

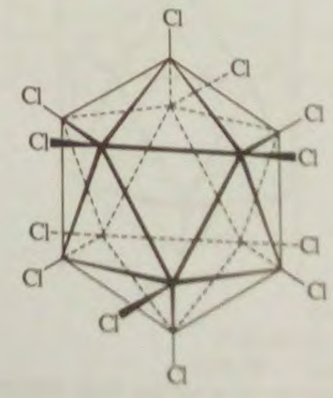
Knoth, W.H. *et al, Inorg. Chem.*, 1964, **3**, 159 (*synth, uv, ir, B-11 nmr, electrochem*)
Kulikova, L.N. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1976, **21**, 509 (*synth, ir*)
Kuznetsov, N.T. *et al, Inorg. Materials* (*Engl. Transl.*), 1980, **16**, 958 (*thermal anal*)
Leites, L.A. *et al, Spectrochim. Acta, Part A*, 1982, **38**, 1047 (*ir, raman*)

IC-001257

$B_{12}Cl_{12}$

Dodecachlorododecaborane(12), 11Cl

[84879-96-9]



M 555.1

Not isol. pure. Subl. ~80°.

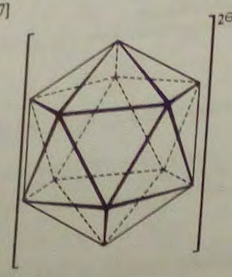
Awad, S.B. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 395 (*synth*)
Massey, A.G., *Adv. Inorg. Chem. Radiochem.*, 1983, **26**, 1 (*rev*)
Saulys, D.A. *et al*, *Inorg. Chem.*, 1983, **22**, 1821 (*synth, ms, B-11 nmr*)

IC-001258

$B_{12}H_{12}^{2\ominus}$

Dodecahydrododecaborate(2−), 11CI, 10CI, 9CI, 8CI

[12356-13-7]



M 141.8 (ion)
closo-. Salts are remarkably stable to chemical attack.

Di-Na salt: [12008-78-5].
$B_{12}H_{12}Na_2$ M 187.8
Colourless cryst. (H_2O). V. sol. H_2O. Anhyd. compd. formed from tetrahydrate at > 195°.

Di-H_3O compd.: Dodecahydrododecaboric acid
$B_{12}H_{18}O_2$ M 179.8
Colourless solid + $2H_2O$. Hygroscopic. Sol. H_2O. Stronger acid than H_2SO_4.

Bis-Et_3NH salt: Colourless needles (dil. aq. HCl). Insol. H_2O. Mp 298-300° dec.

Wunderlich, J.A. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 4427 (*cryst struct*)
Muetterties, E.L. *et al*, *Inorg. Chem.*, 1964, **3**, 444 (*synth, ir, pmr, B-11 nmr, tox, electrochem*)
Inorg. Synth., 1967, **10**, 88 (*synth, ir*)
Kuznetsov, N.T. *et al*, *Inorg. Materials* (*Engl. Transl.*), 1978, **14**, 1567 (*thermal anal*)
Srebny, H.-G. *et al*, *Z. Naturforsch., B*, 1984, **39**, 189 (*ir, raman, B-11 nmr*)

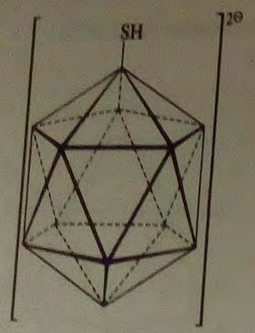
IC-001259

$B_{12}H_{12}S^{2\ominus}$

Mercaptoundecahydrododecaborate(2−)

Undecahydromercaptododecaborate(2−), 10CI, 9CI, 8CI

[12294-22-3]



M 173.8 (ion)

Di-Na salt: [12448-24-7].
$B_{12}H_{12}Na_2S$ M 219.8
Investigated for use in treating brain tumours.
Colourless cryst. Sol. H_2O.

Di-Cs salt: [12448-23-6].
$B_{12}Cs_2H_{12}S$ M 439.7
Colourless cryst. (H_2O). Sol. H_2O.

Knoth, W.H. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 3973 (*synth, ir*)
Shiro, M. *et al*, *Chem. Ind.* (*London*), 1970, 564 (*cryst struct*)
Wellum, C.R. *et al*, *Inorg. Chem.*, 1977, **16**, 2120 (*synth, raman, B-11 nmr*)
Tolpin, E.I. *et al*, *Inorg. Chem.*, 1978, **17**, 2867 (*synth*)
Slatkin, D. *et al*, *Biochem. Pharmacol.*, 1986, **35**, 1771 (*pharmacol*)

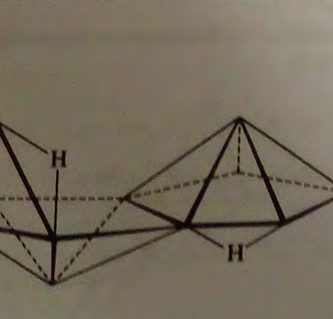
IC-001260

$B_{12}H_{12}S_2^{2\ominus}$

1,2,3,4,5,6,7,8,10,12-Decahydro-9,11-dimercaptododecaborate(2−), 10CI

1,7-Dimercapto-2,3,4,5,6,8,9,10,11,12-decahydrododecaborate(2−)

[67350-74-7]



M 205.9 (ion)
closo-. Detected as a mixt. of isomers in soln.

Tolpin, E.I. *et al*, *Inorg. Chem.*, 1978, **17**, 2867 (*synth, B-11 nmr*)

IC-001261

$B_{12}H_{14}O_{29}Zn_4$

Tetrazinc dodecaborate heptahydrate

Boron zinc oxide ($B_6Zn_2O_{11}$), *hydrate, 11CI, 10CI, 9CI*

[12447-61-9]

$4ZnO.6B_2O_3.7H_2O$

M 869.3
Struct. unknown. Commercially available as fire retardant compd. Used in plastics. Colourless solid. Spar. sol. H_2O. Retains H_2O molecules to temps. below 250°.

[12280-02-3, 12447-61-9, 12513-27-8]

Fr. Pat., 1 560 173, (1969); *CA*, 1969, **71**, 83098.
U.S. Pat., 3 549 316, (1970); *CA*, 1970, **72**, 23010.

IC-001262

$B_{12}H_{16}$

Dodecaborane(16)

Hexaborano(10)[2',3':3,8]octaborane(12), 11CI

[89711-39-7]

M 145.8

Formally *nido-*; *conjuncto*-struct. Synth. from KB_6H_9 + $FeCl_2$ + $FeCl_3$ in Et_2O at −78°. Air stable colourless cryst. by subl. Sol. C_6H_6, hexane. Mp 64-66° dec.

Brewer, C.T. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 2722; 1985, **107**, 3558 (*synth, ir, ms, pmr, B-11 nmr, cryst struct*)

IC-001263

$B_{12}I_{12}^{2\ominus}$

Dodecaiododecaborate(2−), 11CI, 10CI, 9CI, 8CI

[52502-72-4]

As Dodecabromododecaborate(2−), IC-001251 with

X = I

M 1652.5 (ion)
closo-.

Bis-H_3O compd.: Dodecaiododecaboric acid
$B_{12}H_6I_{12}O_2$ M 1690.6
Cryst. + $3H_2O$. Sol. H_2O, Me_2CO, MeOH.

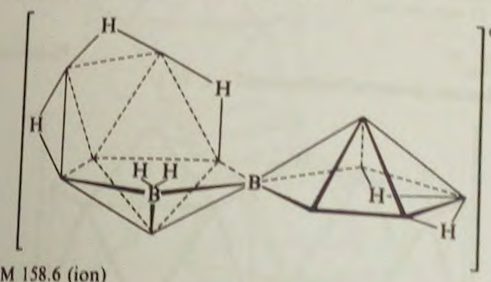
Bis-Me_4N salt: [39422-91-8].
Colourless solid. Sol. aq. MeCN.

Knoth, W.H. *et al*, *Inorg. Chem.*, 1964, **3**, 159 (*synth, uv, ir, B-11 nmr*)
Kulikova, L.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1976, **21**, 509 (*synth, ir*)
Kuznetsov, N.T. *et al*, *Inorg. Materials* (*Engl. Transl.*), 1980, **16**, 958 (*thermal anal*)
Leites, L.A. *et al*, *Spectrochim. Acta, Part A*, 1982, **38**, 1047 (*ir, raman*)

IC-001264

$B_{13}H_{18}^{\ominus}$

Octadecahydrotridecaborate(1−), 9CI



M 158.6 (ion)
Formally *arachno-*; *conjuncto*-struct.

K salt: [56363-22-5].
Yellow solid. Sol. MeCN, Et_2O.

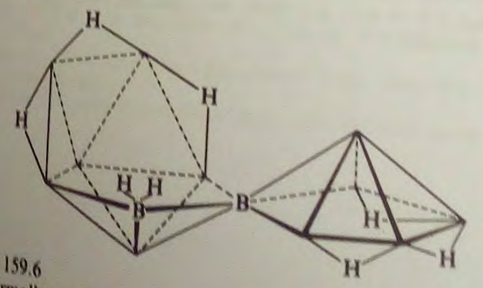
Huffman, J.C. *et al*, *Inorg. Chem.*, 1976, **15**, 227 (*synth, B-11 nmr*)

IC-001265

$B_{13}H_{19}$

Tridecaborane(19), 10CI, 9CI

[43093-20-5]



M 159.6
Formally *arachno-*; *conjuncto*-struct. Yellow cryst. Sol. hexane, CH_2Cl_2. Mp 43.5-44°.

Huffman, J.C. *et al*, *Inorg. Chem.*, 1973, 308 (*cryst struct*)
Rathke, J. *et al*, *Inorg. Chem.*, 1974, **13**, 3040 (*synth, B-11 nmr*)
Huffman, J.C. *et al*, *Inorg. Chem.*, 1976, **15**, 227 (*synth, uv, ms, B-11 nmr, cryst struct*)
Dolan, P.J. *et al*, *Inorg. Chem.*, 1981, **20**, 745 (*synth*)

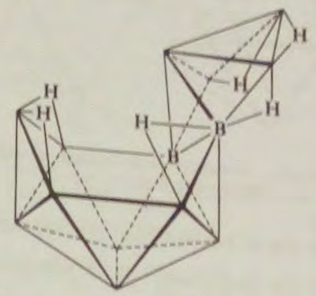
IC-001266

$B_{14}H_{18}$

Tetradecaborane(18), 9CI

Hexaborano(10)[2,3':5,6]decaborane(14), 9CI

[55606-55-8]



M 169.4
Formally *nido-*; *conjuncto nido*-B_{10} and *nido*-B_6 structure. Viscous, pale yellow oil, air-sensitive, stable to H_2O. Sol. cyclohexane, CS_2. $Bp_{0.0001}$ 50°.

[37280-53-8]

Hermanek, S. *et al*, *Chem. Ind.* (*London*), 1972, 606 (*synth, ir, uv, B-11 nmr, ms*)
Hermanek, S. *et al*, *Inorg. Chem.*, 1975, **14**, 2250 (*synth, ir, uv, B-11 nmr, ms*)

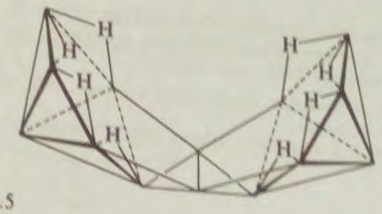
IC-001267

$B_{14}H_{20}$

Tetradecaborane(20)

Octaborano(12)[8',3':3,8]octaborane(12), 10CI, 9CI

[55823-36-4]



M 171.5
Formally *arachno-*; *conjuncto* struct. Mod. air stable yellow cryst.

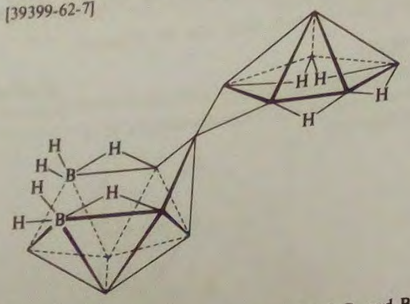
Huffman, J.C. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 1621 (*synth, ms, B-11 nmr, cryst struct*)
Huffman, J.C. *et al*, *Inorg. Chem.*, 1981, **20**, 741 (*synth, ms, B-11 nmr, cryst struct*)

$B_{18}H_{23}$ – $B_{18}H_{20}^{2\ominus}$

IC-001268

$B_{15}H_{23}$
Pentadecaborane(23), 9CI

[39399-62-7]



M 185.3

Formally *hypho-*; *conjuncto*-from linkage of *nido*-B_6 and B_9 species. Sol. $CHCl_3$, CH_2Cl_2.

[51965-60-7]

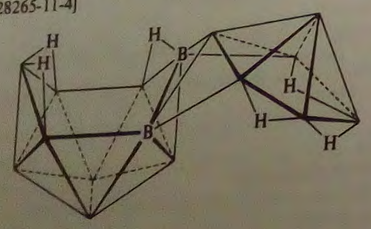
Rathke, J.R. *et al, J. Am. Chem. Soc.*, 1973, **95**, 3402 (*synth, B-11 nmr*)

Rathke, J.R. *et al, Inorg. Chem.*, 1974, **13**, 3008 (*synth, B-11 nmr*)

IC-001269

$B_{16}H_{20}$
Hexadecaborane(20), 10CI, 9CI, 8CI

[28265-11-4]



M 193.1

Formally *nido-*; *conjuncto* from linkage of *nido*-B_{10} and *nido*-B_6 species. Colourless cryst. (pentane). Sol. CCl_4, cyclohexane, THF. Mp 108-112°.

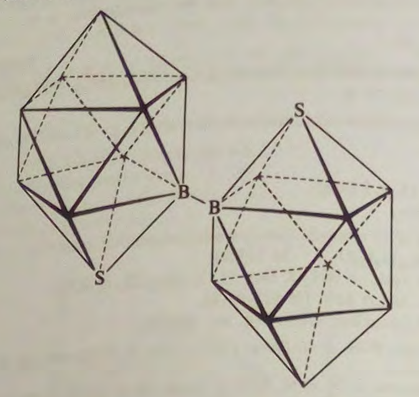
Plesek, J. *et al, Collect. Czech. Chem. Commun.*, 1967, **33**, 699 (*synth, ir, ms, uv*)

Friedman, L.B. *et al, Inorg. Chem.*, 1970, **9**, 1452 (*cryst struct*)

IC-001270

$B_{18}H_{16}S_2$
2,2′-Bi(1-thiadecaborane(9)), 9CI

[54748-44-6]



M 274.8

Two formally *closo*-SB_9 cages joined at 2,2′-positions. Colourless cryst. (CH_2Cl_2). Sol. C_6H_6, heptane, $CHCl_3$. Mp 159.5-161°.

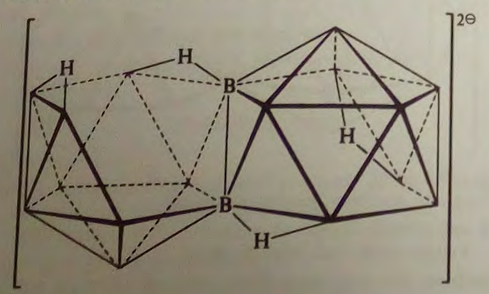
Pretzer, W.R. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 629 (*synth, B-11 nmr, cryst struct*)

Pretzer, W.R. *et al, Inorg. Chem.*, 1975, **14**, 2459 (*cryst struct*)

Pretzer, W.R. *et al, Inorg. Chem.*, 1976, **15**, 1779 (*synth, ir, pmr, B-11 nmr, ms, uv*)

IC-001271

$B_{18}H_{20}^{2\ominus}$
Eicosahydrooctadecaborate(2−), 8CI



M 214.7 (ion)

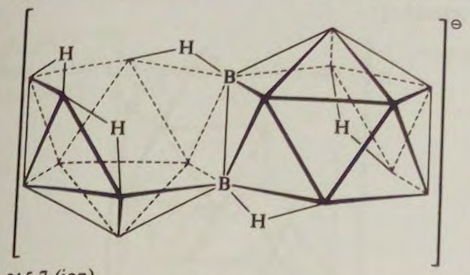
Salts formed from both *n*- and *iso*- $B_{18}H_{22}$.

Bis-Me_4N salt: [12546-32-6].
Pale yellow solid (MeCN).

Olsen, F.P. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3946 (*synth, ir, uv, B-11 nmr*)

$B_{18}H_{21}^{\ominus}$
Heneicosahydrooctadecaborate(1−), 11CI, 8CI

IC-001272



M 215.7 (ion)

n-isomer. Salts obt. from both *n*- and *iso*- $B_{18}H_{22}$.

Me_4N salt: Yellow cryst. (aq. MeCN).

Olsen, F.P. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3946 (*synth, ir, uv, B-11 nmr*)

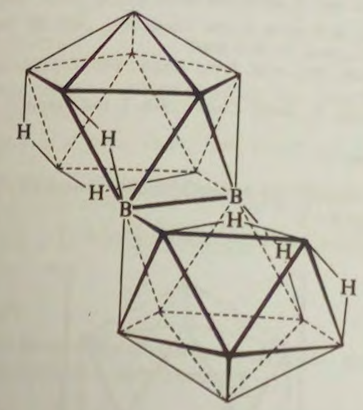
Bould, J. *et al, Polyhedron*, 1983, **2**, 1401 (*synth, B-11 nmr*)

$B_{18}H_{22}$
***n*-Octadecaborane(22)**

IC-001273

(5,7′-μH),(6,7-μH),(8′,9′-μH),(9,10-μH),(9′,10′-μH)[nido-*Decaborano*[6′,5′:5,6]-nido-*decaborane*](22)

[11071-61-7]



M 216.7

n- isomer. Pale yellow cryst. (pentane). Sol. org. solvs. Mp 179-180°.

Pitochelli, A.R. *et al, J. Am. Chem. Soc.*, 1962, **84**, 3128 (*synth, ir, uv*)

Simpson, P.G. *et al, J. Chem. Phys.*, 1963, **39**, 26 (*cryst struct*)

Plesek, J. *et al, Collect. Czech. Chem. Commun.*, 1967, **32**, 1095 (*synth*)

Olsen, F.P. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3946 (*synth, uv, B-11 nmr*)

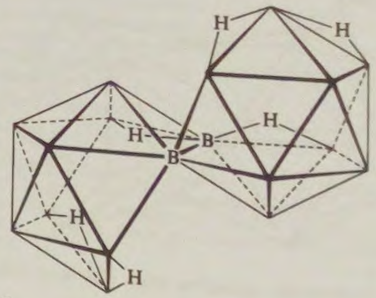
McAvoy, J.S. *et al, J. Chem. Soc., Dalton Trans.*, 1969, 1378 (*synth, uv, ms*)

Gaines, D.F. *et al, J. Am. Chem. Soc.*, 1984, **106**, 7266 (*synth*)

IC-001274

$B_{18}H_{22}$
***iso*-Octadecaborane(22)**

[25037-30-3]



M 216.7

iso- isomer. Solid. Sol. cyclohexane. Mp 128-129°. Can be resolved into its enantiomers.

Pitochelli, A.R. *et al, J. Am. Chem. Soc.*, 1962, **84**, 3218 (*synth, ir, uv*)

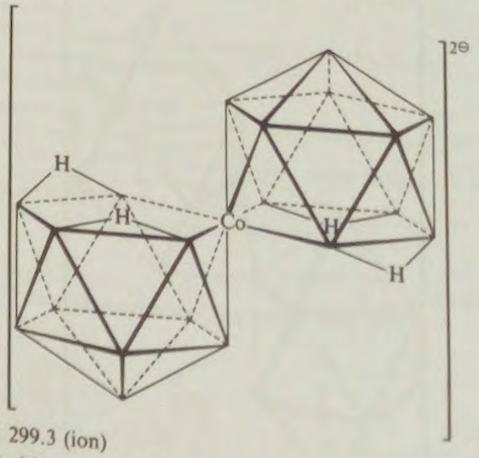
Simpson, P.G. *et al, J. Chem. Phys.*, 1963, **39**, 2339 (*cryst struct*)

Olsen, F.P. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3946 (*synth, uv, B-11 nmr*)

Hermanek, S. *et al, Collect. Czech. Chem. Commun.*, 1970, **35**, 2488 (*ir, uv, resol*)

$B_{20}CoH_{24}^{2\ominus}$
Bis[(1,2,3,6-η)-dodecahydrodecaborato(2−)]cobaltate(2−)

IC-001275



M 299.3 (ion)

Bis-Me_4N salt: [31388-26-8].
Red needle-like cryst. Sol. toluene. Mp 140° dec.

Klanberg, F. *et al, Inorg. Chem.*, 1968, **7**, 2072 (*synth, B-11 nmr*)

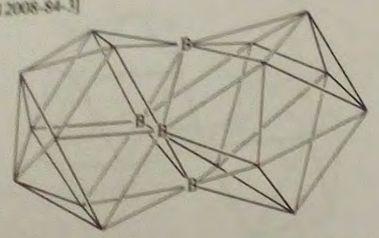
IC-001276

$B_{20}H_{16}$

Eicosaborane(16), 10CI, 9CI, 8CI

Icosaborane(16)

[12008-84-3]



M 232.3

closo-. Hygroscopic colourless cryst. Sol. most org. solvs. Mp 196-199°.

[59458-35-4]

Friedmann, L.B. *et al, J. Am. Chem. Soc.*, 1963, **85**, 3505 (*synth, B-11 nmr*)

Miller, N.E. *et al, J. Am. Chem. Soc.*, 1963, **85**, 3506 (*synth, ir, ms, B-11 nmr*)

Miller, N.E. *et al, Inorg. Chem.*, 1964, **3**, 1690 (*synth, ir, ms, pmr, B-11 nmr*)

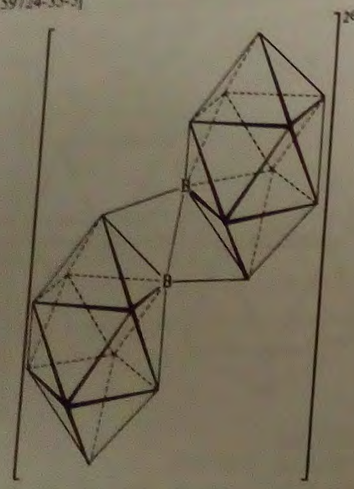
Dobrott, R.D. *et al, J. Chem. Phys.*, 1964, **40**, 866 (*cryst struct*)

IC-001277

$B_{20}H_{18}^{2\ominus}$

Octadecahydroeicosaborate(2−), 10CI, 9CI, 8CI

[59724-35-5]



M 234.3 (ion)

conjuncto ion from linkage of two *closo*-B_{10} species.

Bis-Me_4N salt: [12074-02-1].
Yellow cryst. (aq. MeCN). Sol. H_2O.

Bis-Et_3NH salt: [12404-15-8].
Sol. H_2O.

Chamberland, B.L. *et al, Inorg. Chem.*, 1964, **3**, 1450 (*synth, uv, ir, B-11 nmr*)

Pilling, R.L. *et al, J. Am. Chem. Soc.*, 1964, **86**, 3568 (*B-11 nmr*)

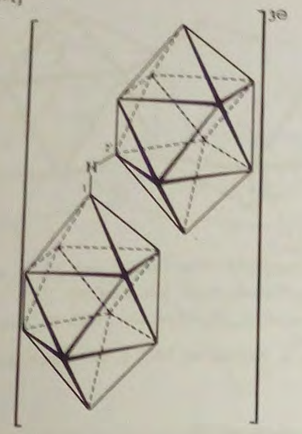
Schwalbe, C.H. *et al, J. Am. Chem. Soc.*, 1969, **91**, 194 (*cryst struct*)

IC-001278

$B_{20}H_{19}^{3\ominus}$

1,2′-Nonadecahydroeicosaborate(3−), 8CI

[12524-07-1]



M 235.3 (ion)

conjuncto ion from linkage of two *closo*-B_{10} species.

Tri-K salt: Colourless solid. Sol. H_2O.

Tris-Me_4N salt: Colourless solid (H_2O). Insol. MeCN.

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1963, **85**, 3704; 1965, **87**, 1893 (*synth, ir, B-11 nmr*)

Chamberland, B.L. *et al, Inorg. Chem.*, 1964, **3**, 1450 (*synth, ir, B-11 nmr*)

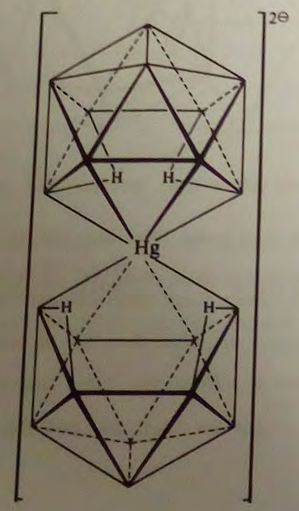
Kaczmarczyk, A., *Inorg. Chem.*, 1968, **7**, 164 (*synth*)

IC-001279

$B_{20}H_{24}Hg^{2\ominus}$

Bis[(5,6,7,8,9,10-η)-dodecahydrodecaborato(2−)]mercurate(2−)

Bis[decaborane(14)-6,9-diyl]mercurate(2−)



M 441.0 (ion)

nido-; the two $B_{10}H_{22}$ moieties are mutually staggered.

Bis-Me_4N salt: [36704-81-1].
Orange plates (Me_2CO aq.).

Bis-$MePh_3P$ salt: [36682-53-8].

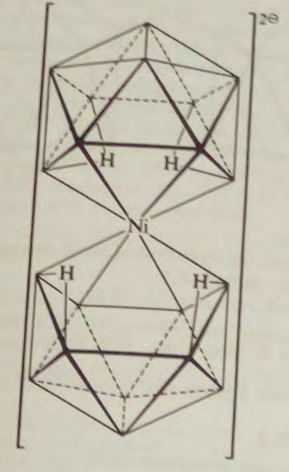
Yellow needles (Me_2CO aq.).

Greenwood, N.N. *et al, J. Chem. Soc. A*, 1971, 3257 (*synth, uv, ir, B-11 nmr, conductivity*)

IC-001280

$B_{20}H_{24}Ni^{2\ominus}$

Bis[(1,2,3,6-η)-dodecahydrodecaborato(2−)]nickelate(2−), 9CI



M 299.1 (ion)

Bis-Me_4N salt: [11141-32-5].
Orange-red cryst. (EtOH/MeCN). Sol. MeCN, H_2O. Mp 180° dec.

Klanberg, F. *et al, Inorg. Chem.*, 1968, **7**, 2072 (*synth, ir, B-11 nmr*)

Guggenberger, L.J., *J. Am. Chem. Soc.*, 1972, **94**, 114 (*cryst struct*)

Siedle, A.R. *et al, Inorg. Chem.*, 1974, **15**, 2838 (*synth*)

Siedle, A.R. *et al, J. Magn. Reson.*, 1978, **31**, 203 (*pmr*)

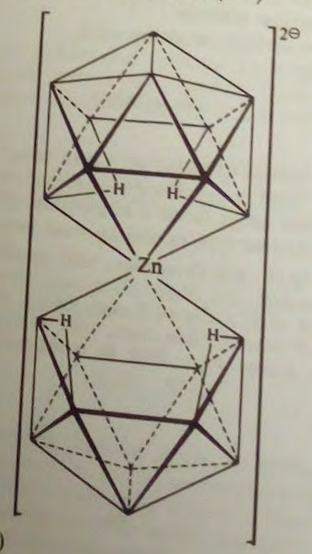
Gaines, D.F. *et al, J. Chem. Soc., Chem. Commun.*, 1982, 122 (*synth*)

IC-001281

$B_{20}H_{24}Zn^{2\ominus}$

Bis[(5,6,9,10-η)-dodecahydrodecaborato(2−)]zincate(2−)

Bis[decaborane(14)-6,9-diyl]zincate(2−)



M 305.8 (ion)

nido-.

Bis-Me_4N salt: [19154-53-1].
Yellow needles (MeOH/Me_2CO). Dec. at 300°.

Bis-$MePh_3P$ salt: Yellow prisms.

Bis[bis(η⁵-2,4-cyclopentadien-1-yl)(2-propanone)(tetrahydrofuran)titanium(1+)] salt:
$C_{54}H_{72}B_{20}O_4Ti_2Zn$ M 922.3
Green paramagnetic cryst. (Me_2CO/THF). Forms solvate with THF.

[36704-82-2, 81900-90-5]

Klanberg, F. *et al, Inorg. Chem.*, 1968, **7**, 2072 (*B-11 nmr, synth, uv*)

Greenwood, N.N. *et al, J. Chem. Soc. A*, 1968, 15; 1971, 809, 3257 (*synth, ir, cryst struct, B-11 nmr, uv, conduct*)

Allmann, R. *et al, Z. Naturforsch., B*, 1976, **31**, 1329 (*cryst struct*)

Gaines, D.F. *et al, J. Chem. Soc., Chem. Commun.*, 1982, 122 (*synth*)

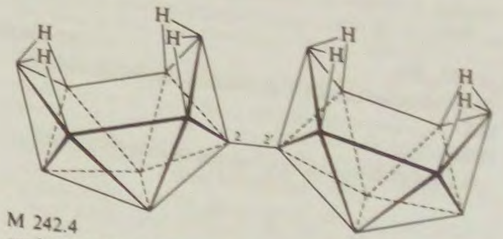
IC-001282

$B_{20}H_{26}$

2,2′-Bidecaborane(14), 11CI, 10CI

Eicosaborane(26), 10CI, 9CI

[71275-37-1]



M 242.4

conjuncto-nido $B_{10}H_{13}$. Colourless cryst. (Et_2O). Sol. common org. solvs. Mp 178-179°.

[51680-89-8]

Greenwood, N.N. *et al, J. Chem. Soc., Chem. Commun.*, 1979, 17 (*synth, B-11 nmr, cryst struct*)

Greenwood, N.N. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 840 (*synth, ms, uv, B-11 nmr*)

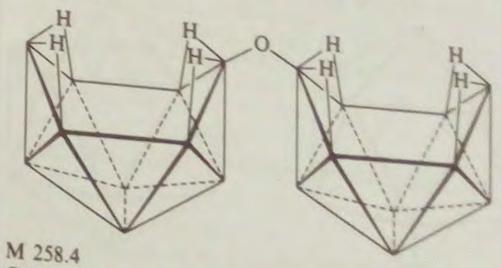
Boocock, S.K. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 790; 1981, 1430 (*pmr, ir, cryst struct, synth, pmr, B-11 nmr*)

IC-001283

$B_{20}H_{26}O$

6,6′-Oxybisdecaborane(14), 11CI, 10CI, 8CI

[17702-42-0]



M 258.4

Colourless cryst. Sol. org. solvs. Mp 137-139°.

Plesek, J. *et al, Collect. Czech. Chem. Commun.*, 1968, **33**, 391 (*synth, ir*)

Kennedy, J.D. *et al, Inorg. Chim. Acta*, 1980, **38**, 93 (*pmr, B-11 nmr*)

Greenwood, N.N. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1251 (*ms, cryst struct*)

Bonnetot, B. *et al, Inorg. Chim. Acta*, 1985, **105**, L15 (*synth*)

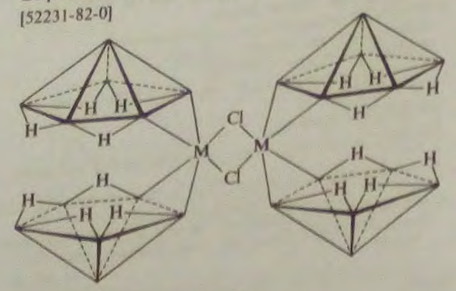
Greenwood, N.N. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 953 (*pmr, B-11 nmr*)

IC-001284

$B_{24}Cl_2H_{40}Ir_2$

Di-μ-chlorotetrakis[(4,5-η)-hexaborane(10)]diiridium, 9Cl

[52231-82-0]



M = Ir

M 755.1

conjuncto-nido-. Orange air-sensitive solid. Mp >90° dec.

Davison, A. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 2802 (*synth, ir, deriv*)

IC-001285

$B_{24}Cl_2H_{40}Rh_2$

Di-μ-chlorotetrakis[(4,5-η)-hexaborane(10)]dirhodium, 9Cl

[52269-70-2]

As Di-μ-chlorotetrakis[(4,5-η)-hexaborane(10)]diiridium, IC-001284 with

M = Rh

M 576.4

conjuncto-nido-. Proposed struct. shown. Orange-red air-sensitive solid; thermally- and air-sensitive in soln. Mp >90° dec.

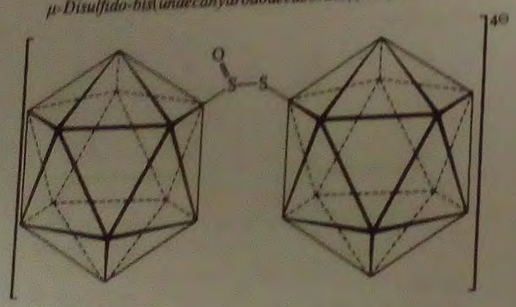
Davison, A. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 2802 (*synth, ir, deriv*)

IC-001286

$B_{24}H_{22}OS_2^{4\ominus}$

1,1′-[μ-[Monothiosulfoxylato(2−)-*S*:*S*′]]bis[2,3,4,5,6,7,8,9,10,11,12-undecahydrododecaborate(4−)], 10Cl

μ-Disulfido-bis(undecahydrododecaborate)(4−) S-oxide



M 361.7 (ion)

Tetrakis-Me_4N salt: [67382-25-6].
Colourless cryst. + $1H_2O$ (H_2O). Sol. H_2O.

Tolpin, E.I. *et al*, *Inorg. Chem.*, 1978, **17**, 2867 (*synth, ir, B-11 nmr*)

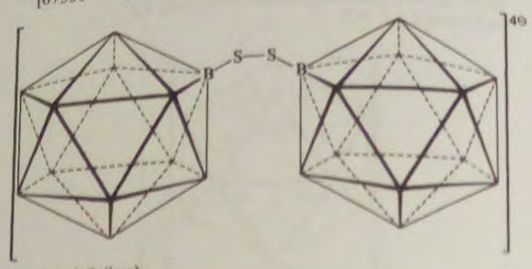
IC-001287

$B_{24}H_{22}S_2^{4\ominus}$

1,1′-Dithiobis[2,3,4,5,6,7,8,9,10,11,12-undecahydrododecaborate](4−), 11Cl, 10Cl

μ-Disulfido-bis(undecahydrododecaborate)(4−)

[67350-75-8]



M 345.7 (ion)

Potential agent for treatment of brain tumours.

Tetra-Na salt: [62962-06-5].
Obt. in soln.; not isol. Sol. H_2O.

Wellum, G.R. *et al*, *Inorg. Chem.*, 1977, **16**, 2120 (*synth*)
Tolpin, E.I. *et al*, *Inorg. Chem.*, 1978, **17**, 2867 (*synth, ir, raman, B-11 nmr*)
Slatkin, D. *et al*, *Biochem. Pharmacol.*, 1986, **35**, 1771 (*pharmacol*)

IC-001288

$[Ba_{0.5}BiK_{0.5}O_3]$

Barium bismuth potassium oxide

[119129-99-6]

$Ba_{1-x}K_xBiO_3$

Sample formula given. Prepd. by heating BaO + KO_2 + BiO_3. High-temp. superconductor when $x \geq 0.37$ with the highest transition temp. 30K. Has a perovskite struct.

[118145-70-3]

Cava, R.J. *et al*, *Nature (London)*, 1988, **332**, 814 (*synth, props*)
Weller, M.T. *et al*, *Physica C (Amsterdam)*, 1988, **156**, 265 (*struct*)
Sleight, A.W., *Science (NY)*, 1988, **242**, 1517 (*rev*)
Pei, S. *et al*, *Phys. Rev. B*, 1990, **41**, 4126 (*phase diagram*)

IC-001289

$Ba_{0.5}NbO_3Sr_{0.5}$

Strontium barium niobate

SBN. Barium niobium strontium oxide

[108158-89-0]

$(Sr,Ba)NbO_3$

M 253.3

A tungsten-bronze ferroelectric. Listed under sample formula. Used in pyroelectric detectors. Over a wide composition range forms a single-phase solid soln. of tungsten-bronze type exhibiting weak ferroelectricity.

Francombe, M.H., *Acta Crystallogr.*, 1960, **13**, 131 (*struct, ferroelectricity*)
Ballman, A.A. *et al*, *J. Crystal Growth*, 1967, **1**, 311 (*synth, props*)
Jamieson, P.B. *et al*, *J. Chem. Phys.*, 1968, **48**, 5048 (*cryst struct*)
Glass, A.M., *J. Appl. Phys.*, 1969, **40**, 4699 (*electrical props*)

IC-001290

Ba

Barium

[7440-39-3]

Ba

M 137.3

Atomic No. 56. Ground state electron config. $[Xe]6s^2$. Isol. by Sir Humphrey Davy in 1808. At least 25 isotopes of which 7, ^{130}Ba, ^{132}Ba, ^{134}Ba, ^{135}Ba, ^{136}Ba, ^{137}Ba, ^{138}Ba are naturally occuring (^{137}Ba, and less so, ^{135}Ba, are used in nmr spectroscopy). Abundance 390 ppm (earth's crust), 0.03 ppm (sea water). Struct. normally bcc, but high pressure forms are known. Also undergoes phase transitions at 309° and 495°. Main mineral is barite ($BaSO_4$). Synth. by thermal dec. of $Ba(N_3)_2$, and from BaO + Al or BaO or BaF_2 with H_2. Getter for removal of residual gases in vacuum tubes. Alloyed with steels to improve corrosion wear resistance. Used in conjunction with Cs in thermionic energy convertors. Commercially available. Soft silvery white metal. The bulk metal tarnishes in air forming Ba_3N_2, BaO, $Ba(OH)_2$ and $BaCO_3$. Finely divided metal ignites in air → mainly Ba_3N_2. Dissolves in H_2O forming $Ba(OH)_2$ solns. Sol. $NH_3(l)$ → blue-black soln. Mp 727° (710°). Bp 1640° (1537°). Burns with yellow-green flame.

▷ Compds. are v. toxic. Ignites readily. Reactive towards H_2O and halogenated hydrocarbons, e.g. CCl_4. CQ8370000.

[13981-97-0, 14698-58-9]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1923, **3**, 619 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 30, 1932 (*rev, bibl*)
Berndt, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1972, **11**, 515 (*synth*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 591 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **3**, 457 (*rev, bibl*)
Evers, J. *et al*, *J. Less-Common Met.*, 1981, **81**, 15 (*synth*)
Nunneman, A. *et al*, *J. Phys. B*, 1985, **18**, L337 (*pe*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 117 (*rev*)
Emsley, J., *The Elements*, 2nd. Ed., Clarendon Press, Oxford, 1991, 26.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 340 (*tox, haz*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 78 (*haz*)

$BaBe_2O_7Si_2$

IC-001291

Barylite, 9CI

[14635-78-0]

$Ba[Be_2Si_2O_7]$

M 323.5

Rare mineral. A framework silicate. Found in limestone at a few specific sites in USA, Canada, Norway, Sweden, and USSR. Colourless white or bluish orthorhombic cryst.

Heinrich, F.W. *et al*, *Am. Mineral.*, 1962, **47**, 758 (*occur*)
Nickel, E.H. *et al*, *Am. Mineral.*, 1962, **47**, 764 (*mineral*)
Robinson, P.D. *et al*, *Am. Mineral.*, 1977, **62**, 167 (*cryst struct*)

$BaBi_{0.5}Pb_{0.5}O_3$

IC-001292

Barium bismuth lead oxide ($BaBi_xPb_{1-x}O_3$)

Barium lead bismuth oxide

[107067-61-8]

$BaPb_{1-x}Bi_xO_3$

M 393.4

Listed under sample formula. Synth. by heating appropriate mixts. of oxides, carbonates or nitrates in air at 800-1000°. Black ($x \leq 0.3$) or bronze-like ($x > 0.3$). Superconductor with highest transition temp. 13K. Struct. is a sl. distorted perovskite.

[110687-39-3]

Sleight, A.W. *et al*, *Solid State Commun.*, 1975, **17**, 27 (*synth, props*)
Battlog, B., *Physica B+C (Amsterdam)*, 1984, **126**, 275 (*superconductivity*)

$BaBiO_3$

IC-001293

Barium bismuthate ($BaBiO_3$)

Bismuthate(2−), barium salt (1:1). Bismuthate ($BiO_3^{3\ominus}$), barium salt. Barium bismuth oxide ($BaBiO_3$)

[12785-50-1]

$BaBiO_3$

M 394.3

Oxidation state(s) of Bi not established, although evidence favours mixed Bi(*III*), Bi(*V*) rather than Bi(*IV*). Monoclinic lattice becoming rhombohedral at ca. 130° and cubic at ca. 580-630°. At r.t., two sets of Bi atoms in perovskite-like struct. Synth. from eg. $Ba(NO_3)_2$ + Bi_2O_3 at 550°. Bronze-coloured cryst. Mp 1040° (incongr.). An insulator which with Pb_3O_4 → superconductors $BaPb_{1-x}Bi_xO_3$.

Sleight, A.W. *et al*, *Solid State Commun.*, 1975, **17**, 27 (*props, use*)
Thornton, G. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 351 (*synth, cryst struct*)
Cox, D.E. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 1 (*synth, cryst struct*)
Thanh, T.D. *et al*, *Appl. Phys.*, 1980, **22**, 205 (*synth, use*)
Shevchuk, A.V. *et al*, *Zh. Neorg. Khim.*, 1985, **30**, 1519; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 866 (*synth, struct*)
Hegde, M.S. *et al*, *Phys. Rev. B*, 1988, **38**, 4557; 1989, **39**, 4752 (*us, struct*)
Skorikov, V.M. *et al*, *Zh. Neorg. Khim.*, 1988, **33**, 2467; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1988, **33**, 1413 (*ir, pe, struct*)

$BaBr_2$

IC-001294

Barium bromide ($BaBr_2$), 8CI

Barium dibromide

[10553-31-8]

$BaBr_2$

M 297.1

$PbCl_2$ type struct. Prepd. by slow neutralisation of $BaCO_3$ with aq. HBr. Cryst. as hydrate. Thermal dec. affords anhyd. product. Forms solid solns. with other alkaline earth metal halides which, when activated with Eu(2+), are used as image recording, storage and conversion systems. Colourless, orthorhombic cryst. V. sol. H_2O (104 g per 100 cm^3 at 20°; 149 g per 100 cm^3 at 100°), EtOH, MeOH. Mp 857°. ΔH_f° −758 kJ mol^{-1}; ΔG_f° −738 kJ mol^{-1}; S° 149 J K^{-1} mol^{-1}.

▷ Highly toxic, irritant.

Monohydrate: [33429-48-0].
Colourless, orthorhombic cryst.; dec. on heating with H_2O loss.

Dihydrate: [7791-28-8].
$BaBr_2H_4O_2$ M 333.1
Cryst. from aq. solns. of $BaBr_2$. Commercially availbale. Colourless, monoclinic cryst.; dec. on heating with H_2O loss (−H_2O at 75°; −$2H_2O$ at 120°). V. sol. H_2O (151 g per 100 cm^3 at 20°; 204 g per 100 cm^3 at 100°), EtOH, MeOH. ΔH_f° −1366 kJ mol^{-1}; ΔG_f° −1231 kJ mol^{-1}; S° 226 J K^{-1} mol^{-1}.

▷ Highly toxic, irritant.

Brackett, E.B. *et al*, *J. Phys. Chem.*, 1963, **67**, 2132 (*cryst struct*)
Swanson, H.E. *et al*, *NBS Monogr. (U.S.)*, 1964, **3**, 10 (*monohydrate, cryst struct*)

Volkov, A.F. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1973, **211**, 1377 (*nqr, dihydrate*)
Lutz, H.D. *et al, Z. Naturforsch., B*, 1973, **28**, 8 (*hydrates, synth, thermal anal*)
Lutz, H.D. *et al, J. Raman Spectrosc.*, 1978, **7**, 130 (*dihydrate, ir, raman*)
Flor, G. *et al, Z. Naturforsch., A*, 1979, **34**, 437 (*dihydrate, thermal dec*)
Lutz, H.D. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 437 (*dihydrate, cryst struct*)
Lutz, H.D. *et al, J. Mol. Struct.*, 1982, **96**, 61; 1983, **101**, 199 (*monohydrate, ir, raman*)
Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 322 (*thermochem data*)
Japan. Pat., 60 84 381, (1985); *CA*, **103**, 62706 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **7**, 333A.

IC-001295

$BaBr_2O_6$
Barium bromate(*V*) ($Ba(BrO_3)_2$)
Bromic acid, barium salt, 8CI
[13967-90-3]

$Ba(BrO_3)_2$

M 393.1
Colourless orthorhombic cryst. Dec. on heating with O_2 evolution and $BaBr_2$ formation. ΔH_f° −753 kJ mol^{-1}; ΔG_f° −577 kJ mol^{-1}; S° 243 J K^{-1} mol^{-1}.
▷ EF8715000.
Monohydrate: [10326-26-8].
$BaBr_2H_2O_7$ M 411.1
Cryst. from aq. solns. of $Ba(BrO_3)_2$. Colourless monoclinic cryst. Dec. on heating with H_2O loss (−H_2O at 85°). Mod. sol. H_2O (0.3 g per 100 cm^3 at 0°; 5.7 g per 100 cm^3 at 100°); sol. Me_2CO; insol. EtOH. ΔH_f° −1055 kJ mol^{-1}; ΔG_f° −825 kJ mol^{-1}; S° 293 J K^{-1} mol^{-1}.

Lumme, P. *et al, Suom. Kem. B*, 1962, **35**, 129; *CA*, 1963, **58**, 958d (*thermal dec, anhyd, hydrate*)
Bancroft, G.M. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1545 (*thermal dec*)
Lutz, H.D. *et al, Z. Anorg. Allg. Chem.*, 1976, **423**, 83; 1985, **529**, 46 (*anhyd, synth, ir, raman, hydrate, cryst structs*)
Harada, A. *et al, Phys. Rep. Kumamoto Univ.*, 1977, **3**, 1; *CA*, 1978, **88**, 143907; **88**, 161099 (*nqr, anhyd, hydrate*)
Finching, F.H. *et al, Sep. Sci.*, 1977, **12**, 65; *CA*, **86**, 22405 (*purif*)
Ramaprabhu, S. *et al, Pramana*, 1984, **23**, 141; *CA*, **101**, 182484 (*nqr, hydrate*)
Lutz, H.D. *et al, Spectrochim. Acta, Part A*, 1985, **41**, 637 (*ir, raman, hydrate*)
Eckers, W. *et al, Spectrochim. Acta, Part A*, 1985, **41**, 1321 (*ir, raman, hydrate*)

IC-001296

$BaBr_6Tc$
Barium hexabromotechnetate(*IV*)
[101408-58-6]

$BaTcBr_6$

M 715.6
Synth. from $Ba(TcO_4)_2$ + $BaBr_2$ in HBr. Dark brown cryst. (body centred orthorhombic), hydrolysed by H_2O to TcO_2. Dec. above *ca.* 430°. Sol. HBr, EtOH, Me_2CO; insol. $CHCl_3$, CCl_4, C_6H_6.

Zaitseva, L.L. *et al, Zh. Neorg. Khim.*, 1986, **31**, 331, 2184; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1986, **31**, 187, 1260 (*synth, ir, tga, powder struct*)

IC-001297

$BaCa_2O_9Si_3$
Walstromite
[15809-39-9]

$Ca_2Ba[Si_3O_9]$

M 445.7
Unbranched monocyclosilicate (3 SiO_4 tetrahedra per unit). Mineral. White or colourless cryst. with pink uv fluorescence.

Dent Glasser, L.S. *et al, Am. Mineral.*, 1968, **53**, 9 (*cryst struct*)
Povarennykh, A.S., *Mineral. Zh.*, 1979, **1**, 3 (*ir*)

IC-001298

$BaCa_4H_{22}O_{46}Si_{15}$
Macdonaldite, 9CI
[15007-62-2]

$BaCa_4H_{20}(SiO_3)_{15}.H_2O$

M 1477.0
Mineral. A branched double layer silicate. Alternatively formulated as $BaCa_4Si_{16}O_{36}(OH)_2.10H_2O$. Occurs in sanbornite-bearing metamorphic rocks in California. Small white orthorhombic needles.

Alfors, J.T. *et al, Am. Mineral.*, 1965, **50**, 314 (*occur*)
Camillo, E., *CA*, 1969, **71**, 25460d (*cryst struct*)

IC-001299

$BaCl_2$
Barium chloride ($BaCl_2$), 8CI
Barium dichloride
[10361-37-2]

$BaCl_2$

M 208.2
Synth. by slow neutralisation of aq. $Ba(OH)_2$ with aq. HCl. Cryst. as hydrate which dec. on heating to form the anhydrous product. Anhydrous $BaCl_2$ prepd. by reaction of barium metal with NH_4Cl in liq. NH_3. Commercially available. Component of speciality glasses, including Ir-transmitting glasses. Used to induce artery contraction. Colourless deliquescent orthorhombic cryst. Undergoes orthorhombic to cubic phase transition at 925°. V. sol. H_2O (37.5 g per 100 cm^3 at 26°; 59 g per 100 cm^3 at 100°); prac. insol. EtOH. Mp 963°. Bp 1560°. ΔH_f° −859 kJ mol^{-1}; ΔG_f° −810.4 kJ mol^{-1}; S° 124 J K^{-1} mol^{-1}.
▷ Highly toxic. Irritant. CQ8750000.
Hemihydrate: [66905-91-7].
Monohydrate: [22322-71-0].
$BaCl_2H_2O$ M 226.2
Synth. by partial dehydration of the dihydrate. Dec. on heating with H_2O loss.
▷ Highly toxic.
Dihydrate: [10326-27-9].
$BaCl_2H_4O_2$ M 244.2
Cryst. from aq. solns. of $BaCl_2$. Commercially available. Colourless monoclinic cryst.; dec. on heating by H_2O loss (−$2H_2O$ at 115°). V. sol. H_2O (58.7 g per 100 cm^3 at 100°); prac. insol. EtOH. ΔH_f° −1460 kJ mol^{-1}; ΔG_f° −1297 kJ mol^{-1}; S° 203 J K^{-1} mol^{-1}.
▷ Highly toxic, irritant. CQ8751000.

Brackett, T.E. *et al, J. Phys. Chem.*, 1963, **67**, 2132 (*cryst struct, polymorphs*)
El Saffer, Z.M. *et al, J. Chem. Phys.*, 1966, **45**, 4643 (*pmr, dihydrate*)
Gardner, T.E. *et al, J. Chem. Eng. Data*, 1969, **14**, 281 (*polymorphs*)

Donnay, J.D.H. *et al, Crystal Data, Determinative Tables*, U.S. Dept. of Commerce/NBS/JCPDS, 3rd Edn., 1973, **2**, 0-163 (*cryst struct, monohydrate*)
Iioka, K., *Kagaku Kyoiku*, 1974, **22**, 350; *CA*, 1975, **82**, 142126 (*rev, bibl, dihydrate*)
Hadenfeldt, C. *et al, Z. Naturforsch., B*, 1975, **30**, 165 (*synth*)
Padmanabhan, V.M. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 2290.(*cryst struct, dihydrate*)
Lutz, H.D. *et al, Appl. Spectrosc.*, 1978, **32**, 541 (*ir, raman, dihydrate*)
Lutz, H.D. *et al, Z. Anorg. Allg. Chem.*, 1979, **457**, 84 (*synth, props, hydrates*)
Tanaka, H. *et al, Thermochim. Acta*, 1981, **51**, 97 (*thermal dec, hydrates*)
Stevens, M.J. *et al, Clin. Exp. Pharmacol. Physiol.*, 1982, **9**, 129; *CA*, **97**, 138350 (*uses*)
Lutz, H.D. *et al, J. Mol. Struct.*, 1982, **96**, 61; 1983, **101**, 199 (*ir, raman, monohydrate*)
Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 327 (*thermodyn*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 334B, 334C (*haz*)

IC-001300

$BaCl_2O_6$
Barium chlorate ($Ba(ClO_3)_2$)
Chloric(V) acid, barium salt, 8CI
[13477-00-4]

$Ba(ClO_3)_2$

M 304.2
Prepd. by slow neutralisation of $BaCO_3$ with aq. $HClO_3$. Cryst. as monohydrate. Thermal dec. under vacuum yields anhyd. material. Component of fireworks giving green colouration to flames. Heat stabiliser and antioxidant for synthetic rubbers and pvc's. Colourless, orthorhombic cryst. Mp 414°. ΔH_f° −763 kJ mol^{-1}; ΔG_f° −557 kJ mol^{-1}; S° 231 J K^{-1} mol^{-1}.
▷ Oxidiser, highly toxic. FN9770000.
Monohydrate: [10294-38-9].
$BaCl_2H_2O_7$ M 322.2
Commercially available. Colourless, monoclinic cryst., dec. on heating by H_2O loss (−H_2O at 120°). V. sol. H_2O (27.4 g per 100 cm^3 at 15°; 111.2 g per 100 cm^3 at 100°); spar. sol. EtOH, Me_2CO. ΔH_f° −1069 kJ mol^{-1}.
▷ Oxidiser, highly toxic.

Kartha, G., *Acta Crystallogr.*, 1952, **5**, 845 (*monohydrate, cryst struct*)
Sahini, V.E. *et al, CA*, 1963, **58**, 7517d (*ir*)
Sikka, S.K. *et al, J. Chem. Phys.*, 1968, **48**, 1883 (*monohydrate, cryst struct, nd*)
Sakellaridis, P.U. *et al, J. Mol. Struct.*, 1972, **12**, 99 (*nqr*)
Langier, J. *et al, Phys. Status Solidi A*, 1974, **24**, K67 (*synth, cryst struct*)
Mathieu, J.P., *CA*, 1976, **85**, 102575 (*monohydrate, thermal dec*)
Lutz, H.D. *et al, Z. Anorg. Allg. Chem.*, 1976, **423**, 83 (*monohydrate, synth, thermal dec*)
Pietrzak, J. *et al, Phys. Status Solidi A*, 1977, **41**, K25 (*monohydrate, nqr*)
Japan. Pat., 59 30 839, 84 30 83, (1984); *CA*, **101**, 8541 (*uses*)
Lutz, H.D. *et al, Spectrochim. Acta, Part A*, 1985, **41**, 637 (*monohydrate, ir, raman*)
Eckers, W. *et al, Spectrochim. Acta, Part A*, 1985, **41**, 1321 (*monohydrate, ir, raman*)
Millar, J.M. *et al, J. Am. Chem. Soc.*, 1986, **108**, 5113 (*monohydrate, pmr*)
Krishnan, V. *et al, Z. Naturforsch., A*, 1986, **41**, 338 (*monohydrate, nqr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 334A.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 342.

IC-001301

$BaCl_2O_8$
Barium perchlorate ($Ba(ClO_4)_2$)
Barium chlorate(VII). Perchloric acid, barium salt, 8CI. Chloric(VII) acid, barium salt
[13465-95-7]

$Ba(ClO_4)_2$

M 336.2
Prepd. by solid state reaction of $Ba(NO_3)_2$ with $(NO)ClO_4$. Neutralisation of $BaCO_3$ with aq. $HClO_4$ leads to the trihydrate. Commercially available. Effective desiccant. Used in pyrotechnic compositions as both oxidiser and colourant. Colourless hexagonal cryst. Undergoes polymorphic transitions at 284° and 350°. Dec. on heating forming $BaCl_2$ + O_2. V. sol. H_2O (198.5 g per 100 cm^3 at 25°; 562.3 g per 100 cm^3 at 100°); v. sol. EtOH. Mp 505°. ΔH_f° −800 kJ mol^{-1}; ΔG_f° −535 kJ mol^{-1}; S° 249 J K^{-1} mol^{-1}.
▷ Oxidiser. Potentially explosive when mixed with organic or organometallic compds. Highly toxic. SC7550000.
Monohydrate: [78914-14-4].
Formed during thermal dehydration of trihydrate.
Trihydrate: [10294-39-0].
$BaCl_2H_6O_{11}$ M 390.2
Commercially available. Colourless hexagonal cryst., dec. on heating with H_2O loss. V. sol. H_2O (198 g per 100cm^3 at 33°). EtOH (124 g per 100 cm^3 at 62°).

Markowitz, M.M. *et al, J. Inorg. Nucl. Chem.*, 1960, **16**, 159 (*synth*)
Mani, N.V. *et al, Z. Kristallogr.*, 1960, **114**, 200 (*cryst struct, trihydrate*)
Ross, S.D., *Spectrochim. Acta*, 1962, **18**, 225 (*ir, trihydrate*)
Lumme, P. *et al, Suom. Kem. B*, 1962, **35**, 129 (*synth, thermal dec*)
Chudinova, L.I., *CA*, 1963, **58**, 1114b (*synth, thermal dec*)
Jacobs, P.W.M. *et al, Combust. Flame*, 1971, **17**, 125; *CA*, 1972, **76**, 88022 (*thermal dec*)
Krauzman, M. *et al, Bull. Soc. Fr. Minéral. Cristallogr.*, 1972, **95**, 538; *CA*, 1973, **78**, 141790 (*raman, struct, trihydrate*)
Gazet, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1978, **286**, 609 (*polymorph*)
Lemesheva, D.M., *Zh. Neorg. Khim.*, 1984, **29**, 1402 (*polymorph, rev*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 337B.

IC-001302

$BaCl_6Tc$
Barium hexachlorotechnetate(*IV*) ($BaTcCl_6$)
[104185-51-5]

$BaTcCl_6$

M 448.9
Synth. by reduction of $Ba(TcO_4)_2$ in HCl + $BaCl_2$. Golden-yellow cryst., dec. at *ca.* 440°. Hydrol. to TcO_2 in H_2O. Sol. aq. HCl; spar. sol. EtOH, Me_2CO; insol. CCl_4, C_6H_6.

Zaitseva, L.L. *et al, Zh. Neorg. Khim.*, 1986, **31**, 1388; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1986, **31**, 793 (*synth, ir, tga, powder struct*)
Zaitseva, L.L. *et al, Zh. Neorg. Khim.*, 1987, **32**, 675; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1987, **32**, 378 (*ir, struct*)

IC-001303

$BaCrO_4$
Barium chromate(*VI*) ($BaCrO_4$)
CI Pigment yellow 31. Lemon yellow. Ultramarine yellow. Permanent yellow. CI 77103. Chromate(VI) barium salt (1:1)
[10294-40-3]

$BaCrO_4$

M 253.3
Known since 1809. Manuf. from $BaCl_2$ and Na_2CrO_4. Synth. from e.g. chromic acid and $Ba(OH)_2$. Used in pyrotechnics and high temp. batteries. Pigment for artists' paints, glass, porcelain. Anticorrosive. V. pale yellow cryst. Darkens on heating. Sol. strong acids; insol. org. solvs. Mp ~1400° dec.

▷ CQ8760000.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1931, **11**, 271 (*bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 52, 1962, **B**, 835 (*rev, bibl*)
Allen, G.C. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1675 (*pe*)
Lentz, A. *et al, Cryst. Res. Technol.*, 1986, **21**, 827 (*cryst struct*)

IC-001304

$BaCuO_{10}Si_4$

Barium copper silicate ($BaCu(Si_4O_{10})$)

[16482-38-5]

$BaCu[Si_4O_{10}]$

M 473.2
A sheet silicate, isostructural with gillespite ($BaFeSi_4O_{10}$). Synth. from $BaCO_3$, CuO and amorphous silica. Has been identified as a blue pigment on ancient Chinese pottery. Blue cryst.

Pabst, A., *Acta Crystallogr.*, 1959, **12**, 733 (*synth, cryst struct*)
Clark, M.G. *et al, J. Chem. Soc. A*, 1967, 1034 (*uv-vis*)
Grefer, J. *et al, Z. Naturforsch., A*, 1973, **28**, 464 (*reflectance spect*)
Bayer, G. *et al, Naturwissenschaften*, 1975, **62**, 181 (*synth*)
Fitz Hugh, E.W. *et al, Stud. Conserv.*, 1983, **28**, 15; *CA*, **98**, 178226q (*use*)
Lin, C. *et al, Kuangwu Xuebao*, 1985, **5**, 301; *CA*, 1986, **105**, 12335n (*esr*)

IC-001305

$BaCu_2S_4Sn$

Barium dicopper thiostannate

Barium copper tin sulfide ($BaCu_2SnS_4$). Barium copper tetrathioxostannate, 9CI

[61036-21-3]

$BaCu_2SnS_4$

M 511.3
Trigonal cryst.

Teske, C.L. *et al, Z. Anorg. Allg. Chem.*, 1976, **426**, 281 (*synth, cryst struct*)

IC-001306

BaF_2

Barium fluoride (BaF_2), 8CI

[7787-32-8]

BaF_2

M 175.3
Fluorite struct. Prepd. by reaction of BaO or $BaCO_3$ with NH_4HF_2 or NH_4F. High purity BaF_2 has been obt. by fluorination of $BaCl_2$ at 600-1000° in a pyrocarbon crucible. Commercially available. Component of speciality glasses, including ir-transmitting glasses. Forms solid solns. with wide variety of metal halides. Colourless, cubic cryst. Spar. sol. H_2O (0.12 g per 100 cm^3 at 25°). Mp 1368°. Bp 2137°. ΔH_f° −1209 kJ mol^{-1}; ΔG_f° −1158 kJ mol^{-1}; S° 96.4 J K^{-1} mol^{-1}.

▷ Highly toxic, corrosive. CQ9100000.

Swanson, H.E. *et al, Natl. Bur. Std. Circ. (U.S.)*, 1953, **1**, 70 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 684 (*uses*)
Volynets, F.K. *et al, Zh. Prikl. Khim. (Leningrad)*, 1979, **52**, 458 (*synth*)
Luginina, A.A. *et al, Zh. Neorg. Khim.*, 1981, **26**, 332 (*synth*)
Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 333 (*thermodyn*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 335B.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 344.

IC-001307

BaF_6Si

Barium hexafluorosilicate(*IV*)

Hexafluorosilicate(2−) barium salt, 8CI. Barium fluosilicate

[17125-80-3]

$Ba[SiF_6]$

M 279.4
Comprises $Ba^{2\oplus}$ cations and $SiF_6^{2\ominus}$ anions. Synth. by reaction of aq. H_2SiF_6 with $Ba(OH)_2$ or $BaCO_3$. Manuf. by treatment of H_2SiF_6 vapour with aq. $BaCl_2$ in a contactor. Wood preservative, esp. in combination with pentachlorophenolates. Colourless rhombohedral cryst. Dec. on heating (~430°) to form SiF_4 and BaF_2. Spar. sol. H_2O (0.026 g per 100 cm^3 at 17°; 0.09 g per 100 cm^3 at 100°); insol. EtOH.

▷ Toxic. CR0525000.

Shurvell, H.F., *Can. Spectrosc.*, 1967, **12**, 156 (*ir*)
U.S. Pat., 3 369 863, (1968); *CA*, **68**, 88658 (*manuf*)
Breitinger, D. *et al, J. Solid State Chem.*, 1977, **22**, 233 (*raman*)
Kolditz, L. *et al, Z. Anorg. Allg. Chem.*, 1979, **452**, 54 (*thermal dec*)
Hoskins, B.F. *et al, Inorg. Chim. Acta*, 1984, **88**, 217 (*cryst struct*)
U.S. Pat., 345 458, (1984); *CA*, **100**, 88140 (*synth, dec*)

IC-001308

BaF_9KV_2

Barium potassium tri-μ-fluorohexafluorodivanadate(*III*)

Barium potassium vanadium(III) fluoride ($BaKV_2F_9$)

[85759-43-9]

$BaK[V_2F_9]$

M 449.2
Double chain struct., like that of $KPbCr_2F_9$. Synth. from BaF_2, KF and VF_3. Mp 880°. The BaNa salt is also known.

Vlasse, M. *et al, J. Solid State Chem.*, 1982, **41**, 272 (*analogue, cryst struct*)
de Kozak, A. *et al, Rev. Chim. Minér.*, 1982, **19**, 668 (*synth, cryst struct, magnetism*)

IC-001309

BaF_9NaV_2

Barium sodium tri-μ-fluorohexafluorodivanadate(*III*), 11CI

Barium sodium vanadium fluoride ($BaNaV_2F_9$)

[85759-44-0]

$BaNaV_2F_9$

M 433.1
Has double chain struct. Synth. from BaF_2, NaF and VF_3. Cryst. Mp 816°. Antiferromagnetic, T_N ~6K.

Vlasse, M. *et al, J. Solid State Chem.*, 1982, **41**, 272 (*analogue, cryst struct*)
de Kozak, A. *et al, Rev. Chim. Minér.*, 1982, **19**, 668 (*synth, cryst struct, magnetism*)

IC-001310

$BaFeHMn_2O_9Si_2$

Orthoericssonite

[59055-22-0]

$Ba[FeMn_2(OH)(SiO_4)_2]$ or $(Ba,Sr)(Mn,Fe)_2(Fe,Ti)[Si_2O_7](O,OH)_2$

M 504.2
Mineral. Red-black cryst.

Matsubara, S., *Mineral. J.*, 1980, **10**, 107 (*cryst struct*)

IC-001311

$BaFeO_{10}Si_4$

Barium iron(*II*) silicate ($BaFe(Si_2O_5)_2$)

Gillespite

[16102-62-8]

$BaFe[Si_2O_5]_2$

M 465.5
Mineral. Unbranched single layer silicate. Red; translucent and vitreous cryst. $Fe^{2\oplus}$ ions exhibit effect of spin relaxation. Shows phase transition at 1.8×10^4 atm.

Schaller, W.T., *Am. Mineral.*, 1929, **14**, 319.
Bancroft, G.M. *et al, Pap. Proc. Gen. Meet., Int. Mineral. Assoc., 5th, 1966*, 1968, 36 (*mössbauer*)
Hazen, R.M., *Am. Mineral.*, 1977, **62**, 528 (*phase transition*)
Mackey, D.J. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 299 (*magnetism, electronic struct*)
Srivastava, K.K.P. *et al, Indian J. Phys., A*, 1981, **55**, 299 (*mössbauer, magnetism*)
Srivastava, K.K.P. *et al, Phys. Status Solidi B*, 1982, **113**, 93 (*mössbauer, magnetism*)
Hazen, R.M. *et al, Am. Mineral.*, 1983, **68**, 595 (*struct, phase transition*)
Waychunas, G.A. *et al, Phys. Chem. Miner.*, 1983, **10**, 1 (*uv-vis, struct*)
Belsky, H.L. *et al, Am. Mineral.*, 1984, **69**, 771 (*related struct*)

IC-001312

$BaGa_2Ge_2O_8$

Barium gallium germanium oxide ($BaGa_2Ge_2O_8$)

[50810-86-1]

$BaGa_2Ge_2O_8$

M 549.9
Open framework with 9-coord. Ba and 4-coord. (tetrahedral) Ga, Si. Obt. as both celsian and paracelsian forms. Obt. from oxide melt. Cryst. (melt).

Calleri, M. *et al, Acta Crystallogr., Sect. B*, 1976, **32**, 1196, 2733 (*cryst struct*)
Kroll, H. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 359 (*cryst struct*)

IC-001313

$BaGa_2O_4$

Barium gallium oxide ($BaGa_2O_4$)

[12047-12-0]

$BaGa_2O_4$

M 340.7
Hexagonal superstructure based on tridymite (SiO_2) with Ba in interstices; with tetrahedral Ga and 9-coord. Ba. Synth. from fused Ba_2CO_3—Ga_2O_3 mixt. Colourless cryst. (melt).

Hoppe, R. *et al, Naturwissenschaften*, 1960, **47**, 376 (*cryst struct*)
Glasser, F.P. *et al, J. Am. Ceram. Soc.*, 1963, **46**, 377 (*synth, cryst struct*)
Hoffman, C.W.W. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 63 (*phase diagram*)
Deiseroth, H.-J. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 3177 (*cryst struct*)

IC-001314

$BaGa_2O_8Si_2$

Barium gallosilicate ($BaGa_2Si_2O_8$)

Barium gallium silicate ($BaGa_2Si_2O_8$)

$BaGa_2Si_2O_8$

M 460.9
Open framework with 7-coord. Ba and tetrahedral Ga, Si. Both celsian and paracelsian forms obt. Synth. from oxide melt. White cryst. (melt).

Gazzoni, G., *Z. Kristallogr.*, 1973, **137**, 24 (*synth*)
Calleri, M. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 560; 1976, **32**, 1196, 2733 (*cryst struct*)
Kroll, H. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 359 (*cryst struct*)

IC-001315

$BaGa_2S_4$

Barium gallium sulfide ($BaGa_2S_4$), 9CI

Barium dithiozogallate(1−), 10CI. Barium thiogallate

[12589-46-7]

$BaGa_2S_4$

M 405.0
Prepd. by reaction of $BaGa_2O_4$ with H_2S. White cryst.

Ivanov-Emin, B.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 515 (*synth*)
Eisenmann, B. *et al, Mater. Res. Bull.*, 1982, **17**, 1169 (*cryst struct*)

IC-001316

$BaGa_2Se_4$

Barium gallium selenide ($BaGa_2Se_4$)

[51403-85-1]

$BaGa_2Se_4$

M 592.6
Orthorhombic $SrAl_2Se_4$ struct. related to TlSe. Contains $GaSe_4$ tetrahedra and 8-coord. (square antiprismatic) Ba. Synth. from $BaGa_2$ and Se at 1000°. Beige translucent air- and moisture-sensitive cryst. (melt).

Klee, W. *et al, Z. Anorg. Allg. Chem.*, 1981, **479**, 125 (*synth, cryst struct*)

IC-001317

$BaGa_2Te_4$

Barium gallium telluride ($BaGa_2Te_4$)

[39297-27-3]

$BaGa_2Te_4$

M 787.1
Structure has $GaTe_4$ tetrahedra sharing corners with half filled $BaTe_8$ antiprisms; (related to TlSe). Obt. from stoichiometric amounts of the elements at 1200°. Dark red air- and moisture-sensitive prisms.

Franke, E.R. *et al, Z. Naturforsch., B*, 1972, **27**, 1308 (*synth, props*)

IC-001318

$BaGeO_3$

Barium germanate ($BaGeO_3$)

Barium metagermanate

[12047-14-2]

$BaGeO_3$

M 257.9
Exists as two phases at atm. press. Various high pressure phases also known. Amorphous at r.t. Complex synth. from Ge and Ba propoxides in aq. NH_3.

α-form
Pseudo wollastonite hexagonal ring struct. Converts to β-form at 1180-1200°.

β-form
Orthorhombic struct. with infinite chains of GeO_4 tetrahedra. From amorph. form at 630-660°. Converts to α-form at 1130-1150°.

Liebau, F., *Neues Jahrb. Mineral., Abh.*, 1960, **94**, 1209.
Hilmer, W., *Acta Crystallogr.*, 1962, **15**, 1101 (*high temp form, struct*)
Grebenshchikov, V.I. *et al. Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 1620 (*low temp cryst struct*)
Kher, V.G. *et al. Curr. Sci.*, 1975, **44**, 46 (*cryst struct*)
Ogannesyan, R.M. *et al. Fiz. Khim. Stekla*, 1978, **4**, 561 (*synth*)
Ozima, M. *et al. J. Solid State Chem.*, 1982, **44**, 307 (*cryst struct, high pressure phase*)
Yamaguchi, O. *et al. Polyhedron*, 1983, **2**, 1213 (*synth*)

IC-001319

$BaGeO_2Zn$

Barium zinc orthogermanate
Barium germanium zinc oxide ($BaGeZnO_4$)
[67163-38-6]

$BaZnGeO_4$

M 339.3
Isomorphous with $BaAl_2O_4$. Tetrahedral BeO_4 interspersed with Ge, Zn in a superstructure. Synth. from a stoichiometric melt of Ba, Zn and Ge oxides by Czochralski method. Piezoelectric ≤ 250°. Undergoes several phase transitions.

Dluh, C.D. *et al. Bull. Soc. Fr. Minéral. Cristallogr.*, 1964, **87**, 108 (*cryst struct*)
Takei, H. *et al. J. Mater. Sci.*, 1980, **15**, 2612 (*synth*)
Tsunekawa, S. *et al. Jpn. J. Appl. Phys.*, 1981, **20**, 657 (*phases*)
Iijima, K. *et al. Acta Crystallogr., Sect. B*, 1982, **38**, 1112 (*cryst struct*)
Shiraki, H. *et al. J. Phys. Soc. Jpn.*, 1984, **53**, 456 (*raman*)
Tanba, N. *et al. J. Phys. Soc. Jpn.*, 1985, **54**, 4783 (*ferroelec phase*)
Kikuchi, M. *et al. J. Solid State Chem.*, 1985, **56**, 390 (*em*)

IC-001320

$BaGe_2O_5Ti$

Barium germanium titanium oxide ($BaTiGe_2O_5$)
Barium germanium titanate
[12513-55-2]

$BaTiGe_2O_5$

M 547.0
Ge analogue of benitoite. Synth. from $BaCO_3$, TiO_2 and GeO_2. Stable from 1132-1235° but dissoc. slowly above and below this temp. range.

Robbins, C.R., *J. Am. Ceram. Soc.*, 1960, **43**, 610 (*stability*)
Robbins, C.R. *et al. J. Res. Natl. Bur. Stand. (U.S.)*, 1961, **65A**, 127 (*cryst struct*)

IC-001321

$[BaHO_3Ru]$

Barium ruthenium trioxide-hydrogen system
Barium ruthenate bronze. Barium ruthenate hydride

H_xBaRuO_3

Hydrogen content continuously variable. Formed by absorption of H_2 by $BaRuO_3$ at r.t.

Shelef, M. *et al. J. Inorg. Nucl. Chem.*, 1976, **38**, 99 (*synth*)

IC-001322

$BaHO_4P$

Barium phosphate (BaHPO$_4$)
Barium phosphate (1:1), 9CI, 8CI. Barium monohydrogenphosphate
[10048-98-3]

$BaHPO_4$

M 233.3
Orthorhombic. Each Ba ion coordinated to 10 O atoms, being bonded to form PO_4 tetrahedra by edge sharing and to 2 more by corner sharing. The PO_4 groups are linked by H-bonds into continuous chains. Synth. from BaO in excess H_3PO_4, or Ba^{2+} + $(NH_4)_2HPO_4$ in H_2O. Also from $Ba(NH_4)PO_4$ when heated. Colourless thin plates or flat needles. Loses H_2O at 500° to give the pyrophosphate. Stable to H_2O at 90°.

Burley, G., *J. Res. Natl. Bur. Stand. (U.S.)*, 1958, **60**, 23 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 30, 1960, 492 (*rev, bibl*)
Miller, F.A. *et al, Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Blinc, R. *et al, Phys. Status Solidi B*, 1976, **74**, 425 (*ir, raman*)
Sato, S. *et al, Bull. Chem. Soc. Jpn.*, 1985, **58**, 3513 (*synth, P-31 nmr*)
Turner, G.L. *et al, J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Mudrakovskii, I.L. *et al, J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)

IC-001323

BaH_2

Barium hydride (BaH_2), 8CI
[13477-09-3]

BaH_2

M 139.3
Isotypic with SrH_2 ($PbCl_2$). Manuf. by direct reaction of the elements at high temps. and pressures. Prepd. by reaction of $BaCl_2$ with H_2 in the presence of liq. Na at 383°. Catalyst for polym. of dienes and lactones. Grey orthorhombic cryst. Moisture-sensitive, reacts with H_2O with formation of $Ba(OH)_2$ and H_2. Dec. on heating with evolution of H_2 gas and formation of Sr. Mp 675°. ΔH_f° −179 kJ mol^{-1}; ΔG_f° −132 kJ mol^{-1}.

▷ Toxic.

Zintl, E. *et al, Z. Elektrochem.*, 1935, **41**, 33 (*cryst struct*)
Franzen, H.F. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1977, **11**, 439 (*pe*)
Nicol, A.T. *et al, J. Chem. Phys.*, 1978, **69**, 5211 (*pmr*)
Shen, P. *et al, Huaxue Tongbao*, 1984, 10; *CA*, 1985, **102**, 105112 (*synth*)

IC-001324

BaH_2O_2

Barium hydroxide ($Ba(OH)_2$), 8CI
[17194-00-2]

$Ba(OH)_2$

M 171.3
Normally obt. as various hydrates, esp. octahydrate. Prepd. by thermal dehydration of the hydrates. White powder. Dec. on heating with H_2O loss. Mp 398°. ΔH_f° −946.3 kJ mol^{-1}; ΔG_f° −859.5 kJ mol^{-1}; S° 107 J K^{-1} mol^{-1}.

▷ Highly toxic, corrosive.

Monohydrate: [22326-55-2].
BaH_4O_3 M 189.3
Prep. by thermal dec. of the octahydrate at 110° in a dry nitrogen stream. Commercially available. A monoclinic modification has been cryst. from EtOH.
Trihydrate: [66905-77-9].

Cryst. from the melt obt. by thermal dec. of the octahydrate at 110°. Colourless orthorhombic cryst.
Hexahydrate: [86624-92-9].
$BaH_{12}O_8$ M 279.4
Octahydrate: [12230-71-6].
$BaH_{20}O_{10}$ M 315.4
Commercially available. Colourless, monoclinic cryst., dec. on heating with H_2O loss. Sol. H_2O (5.6 g per 100 cm^3 at 15°; 95 g per 100 cm^3 at 78°); spar. sol. EtOH, insol. Me_2CO. Mp 78°. ΔH_f° −3342 kJ mol^{-1}, ΔG_f° −2793 kJ mol^{-1}; S° 427 J K^{-1} mol^{-1}.

Manohar, H. *et al, Z. Kristallogr.*, 1966, **119**, 367 (*octahydrate, cryst struct*)
Lutz, H.D. *et al, Spectrochim. Acta, Part A*, 1981, **37**, 561 (*hydrates, ir, raman*)
Lutz, H.D. *et al, Thermochim. Acta*, 1981, **44**, 337 (*hydrates, synth, cryst struct, thermal dec*)
Mu, J.J. *et al, Thermochim. Acta*, 1981, **49**, 207 (*hexahydrate, dec*)
Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 939 (*thermodyn*)
Buchmeier, W. *et al, Z. Anorg. Allg. Chem.*, 1986, **538**, 131 (*monohydrate, trihydrate, synth, cryst structs*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 336C

IC-001325

$BaH_2O_4Sn_2$

Barium bis(hydroxyoxostannate)
[86592-74-7]

$Ba[SnO(OH)]_2$

M 440.7
Struct. contains layers of 1 D $\{SnO(OH)\}^\ominus$ ions in *syn* conformation. Pale-yellow monoclinic cryst.

Nesper, R. *et al, Z. Anorg. Allg. Chem.*, 1983, **499**, 109 (*synth, cryst struct*)

IC-001326

$BaH_4O_8P_2$

Barium phosphate ($Ba(H_2PO_4)_2$)
Barium phosphate (1:2), 9CI, 8CI. Barium bis(dihydrogenphosphate)
[13466-20-1]

$Ba(H_2PO_4)_2$

M 331.3
Two forms present in approx. equal amounts during cryst. growth. Orthorhombic with Ba ions coordinated by 8 O (Ba—O 260-297 pm) and between layers of PO_4 tetrahedra (P—O 149-158 pm, OPO 103.6-119.1°) in H-bonded dimers, and triclinic, with open 2-D network of PO_4 linked by Ba—O (nine at 267.6-296.7 pm) bonds. Hydrates have been reported. Synth. from $BaCO_3$, BaO, or $Ba_3(PO_4)_2$ + H_3PO_4. Transparent colourless plates.
[28016-22-0, 84805-44-7]

Gmelin Handbook Inorg. Chem., Syst. No. 30, 1960, 493 (*rev, bibl*)
Brekhunets, A.G. *et al, Zh. Prikl. Spektrosk.*, 1970, **12**, 509; *J. Appl. Spectrosc. USSR* (*Engl. Transl.*), 1970, **12**, 390 (*pmr, struct*)
Kuz'menkov, M.I. *et al, Zh. Neorg. Khim.*, 1972, **17**, 1898; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1972, **17**, 985 (*props*)
Agre, V.M. *et al, Kristallografiya*, 1976, **21**, 722; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1976, **21**, 408 (*cryst struct*)
Gilbert, J.D. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 3533; 1978, **34**, 3309 (*synth, cryst struct*)
Prelesnik, B. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 76 (*cryst struct*)
Durif, A. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 1671 (*cryst struct*)
Lenhert, P.G., *Acta Crystallogr., Sect. B*, 1981, **37**, 1321 (*cryst struct*)

IC-001327

$BaH_4O_8P_2Zn_3$

Barium zinc phosphonate ($BaZn_3(HPO_3)_4$)
Phosphonic acid, barium, zinc (4 / 1 / 3) salt

$Zn_3Ba(HPO_3)_4$

M 668.4
Hexahydrate: [123269-41-6].
Prep. from BaH_2PO_2, $ZnCl_2$ in aq. H_3PO_3. Colourless rods (aq. EtOH). Contains both octahedral $(Zn(OH_2)_6)$ and tetrahedral Zn; 12-coord. Ba $(Ba(OH_2)_8)$. Ba bridges the Zn(1) octahedron and the P(1) tetrahedron.

Cruz-Avila, C.Y. *et al, Inorg. Chem.*, 1989, **28**, 2068 (*synth, thermal anal, cryst struct*)

IC-001328

BaI_2

Barium iodide (BaI_2), 8CI
[13718-50-8]

BaI_2

M 391.1
Struct. type $PbCl_2$. Prepd. directly by reaction of BaH_2 with $[NH_4]I$ in Py. Alternatively obtained by slow neutralisation of $BaCO_3$ with aq. HI. Cryst. as hydrate. Thermal dec. affords anhyd. prod. Forms solid solns. with other alkaline earth metal halides which when activated with Eu(2+), are used in phosphors for radiographic image conversion screens. Deliquescent, colourless, orthorhombic cryst. Light sensitive. V. sol. H_2O (170 g per 100 cm^3 at 0°), EtOH (77 g per 100 cm^3 at 20°). Mp 711°. ΔH_f° −605 kJ mol^{-1}, ΔG_f° −601 kJ mol^{-1}, S° 165.1 J K^{-1} mol^{-1}.

▷ Highly toxic.

Dihydrate: [7787-33-9].
$BaH_4I_2O_2$ M 427.1
Commercially available. Deliquescent, colourless orthorhombic light sensitive cryst., dec. on heating by H_2O loss (−H_2O at 99°, −2H_2O at 539°). V. sol. H_2O (200 g per 100 cm^3 at 15°; 269 g per 100 cm^3 at 100°), mod. sol. EtOH (1.07 g per 100 cm^3 at 15°). ΔH_f° −1217 kJ mol^{-1}.
Hexahydrate: [13477-15-1].
$BaH_{12}I_2O_6$ M 499.2
Colourless, hexagonal light sensitive cryst. (aq. soln.); dec. on heating by H_2O loss. V. sol. H_2O (410 g per 100 cm^3 at 0°), EtOH. Struct. resembles $K_2Pt(SCN)_6$.

Herrmann, Z., *Z. Anorg. Allg. Chem.*, 1931, **197**, 339 (*hexahydrate, cryst struct*)
U.S. Pat., 2 801 899, (1957); *CA*, **51**, 15910b (*synth*)
Brackett, E.B. *et al, J. Phys. Chem.*, 1963, **67**, 2132 (*cryst struct*)
Lutz, H.D. *et al, Angew. Chem., Int. Ed. Engl.*, 1971, **10**, 183 (*hydrates, ir*)
Lutz, H.D. *et al, Z. Naturforsch., B*, 1973, **28**, 8 (*hydrates, synth, thermal anal*)
Spiridonov, V.P. *et al, Chem. Phys. Lett.*, 1981, **77**, 41 (*ed, struct*)
Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 344 (*thermodyn*)
Japan. Pat., 60 84 381, (1985); *CA*, **103**, 62706 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 336A

IC-001329

BaI_2O_6

Barium iodate(V) ($Ba(IO_3)_2$)
Iodic acid, barium salt, 8CI
[10567-69-8]

$Ba(IO_3)_2$

M 487.1

Prepd. by thermal dehydration of the monohydrate under vacuum. Colourless monoclinic cryst., hygroscopic. Dec. on heating with formation of barium periodate. Spar sol. H_2O (0.04 g per 100 cm^3 at 25°). ΔH_f° −1027 kJ mol^{-1}; ΔG_f° −865 kJ mol^{-1}; S° 249 J K^{-1} mol^{-1}.

Monohydrate: [7787-34-0].
Cryst. from aq. solns. of $Ba(IO_3)_2$ obt. by slow reduction of HIO_4 by lactic acid in the presence of $Ba(NO_3)_2$. Colourless monoclinic cryst.; dec. on heating with H_2O loss (−H_2O at 180°). Spar. sol. H_2O; insol. EtOH, Me_2CO. ΔH_f° −1322 kJ mol^{-1}; ΔG_f° −1104 kJ mol^{-1}; S° 297 J K^{-1} mol^{-1}.

Inorg. Synth., 1963, **7**, 13 (*synth, hydrate*)
Jones, A.L., *J. Crystal Growth*, 1973, **20**, 99 (*soly*)
Lutz, H.D. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1975, **79**, 98 (*ir, raman, hydrate*)
Lutz, H.D. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **423**, 83 (*synth, ir, thermal dec, hydrate*)
Petricek, V., *Acta Crystallogr., Sect. B*, 1980, **36**, 2130 (*cryst struct*)
Biswas, P.K. *et al*, *Thermochim. Acta*, 1980, **42**, 91 (*thermal dec, hydrate*)
Shishkin, V.A. *et al*, *J. Mol. Struct.*, 1982, **83**, 349 (*nqr, hydrate*)
Lutz, H.D. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **535**, 31 (*hydrate, cryst struct*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 344.

IC-001330

[BaIn]

Barium indium system

Barium compd. with indium (1:4)

$BaIn_4$ M 596.6
Isotypic with $BaAl_4$. Structure has puckered layers of In with Ba between. Synth. from elements. Air- and moisture-sensitive soft white cryst. (from melt). $BaIn_2$ also known.

Bruzzone, G. *et al*, *Acta Crystallogr., Sect. B*, 1962, **18**, 1081 (*cryst struct*)
Bruzzone, G., *CA*, 1970, **73**, 103005 (*analogues*)

IC-001331

$BaIn_2Te_4$

Barium indium telluride ($BaIn_2Te_4$)

[39297-28-4]

$BaIn_2Te_4$

M 877.3
Structure has $InTe_4$ tetrahedra sharing corners half filled with $BaTe_8$ antiprisms; struct. resembles TlSe. From stoichiometric amounts of the elements at 1200°. Metallic grey air- and moisture-sensitive prisms.

Franke, E.R. *et al*, *Z. Naturforsch., B*, 1972, **27**, 1308 (*synth, props*)

IC-001332

$BaLaMgO_6Ru$

Barium magnesium hexaoxoruthenatelanthanate ($BaMgRuLaO_6$), 10CI

Barium magnesium lanthanum ruthenium hexaoxide. Barium magnesium lanthanum ruthenium oxide ($BaMgLaRuO_6$)

[74511-54-9]

$BaLaMgRuO_6$

M 497.6
Struct. related to Barium lanthanum ruthenium oxide (Ba_2LaRuO_6), IC-001377. Antiferromagnetic solid (T_N ~ 20-40 K). Analogues with Mg replaced by Ni, Co or Zn are also known. All contain Ru(*V*).

Fernandez, I. *et al*, *J. Solid State Chem.*, 1980, **32**, 97 (*mössbauer, magnetism*)

IC-001333

$BaMnO_3$

Barium manganese(*IV*) oxide ($BaMnO_3$), 9CI

[12230-80-7]

$BaMnO_3$

M 240.2
Struct. resembles $CsNiF_3$, with $Mn^{IV}O_6$ octahedra. Synth. from $BaMnO_4$ at 500-1000° under N_2. Yellowish-green. Antiferromagnetic at low temp.

Scholder, R., *Z. Elektrochem.*, 1952, **56**, 879 (*synth*)
Chamberland, B.L. *et al*, *J. Solid State Chem.*, 1969/70, **1**, 506 (*struct*)
Christensen, A.N. *et al*, *J. Solid State Chem.*, 1972, **4**, 131 (*magnetic struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1975, **C2**, 241 (*rev, bibl*)

IC-001334

$BaMnS_2$

Barium manganese sulfide ($BaMnS_2$), 9CI

[11090-05-4]

$BaMnS_2$

M 256.3
Struct. contains MnS_4 tetrahedra. Prepd. from $BaCO_3$ and Mn powder at 1000° in a stream of H_2S.

Schnering, H.G. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **312**, 87 (*synth, struct*)
Schmitz, D. *et al*, *Naturwissenschaften*, 1971, **58**, 322 (*struct*)
Schmitz, D. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **402**, 225 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1976, **C6**, 44 (*rev, bibl*)

IC-001335

$BaMoO_4$

Barium molybdate(*VI*) ($BaMoO_4$)

Barium molybdenum oxide ($BaMoO_4$)

[7787-37-3]

$BaMoO_4$

M 297.2
Contains the tetrahedral $[MoO_4]^{2\ominus}$ ion. Scheelite type lattice. Obt. by combining aq. solns. of sodium or ammonium molybdate and a sol. barium salt or by heating mixed solid oxides. White solid. Reduced by H_2 on heating to give red $BaMoO_3$. Reacts with O_2 at 800-1200° to give yellow Ba_2MoO_5. Electrical conductor. Insol. H_2O. Mp 1480°.

Frevel, L.K. *et al*, *Ind. Eng. Chem., Anal. Ed.*, 1946, **18**, 43 (*struct*)
Bertaut, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1954, **238**, 2173 (*struct*)

IC-001336

BaN_2O_4

Barium nitrite ($Ba(NO_2)_2$)

Nitrous acid, barium salt, 8CI

[13465-94-6]

$Ba(NO_2)_2$

M 229.3
Cryst. from aq. soln. affords the hydrate which is fully dehydrated at 182°. Reagent for converting metal

sulfates to nitrites. Component of pyrotechnic compositions; oxidiser and colourant. Colourless hexagonal cryst. Dec. on heating with intermed. formation of $Ba(NO_3)_2$ and final formation of BaO. Pyroelectric. V. sol. H_2O (67 g per 100 cm^3 at 20°; 300 g per 100 cm^3 at 100°); mod. sol. EtOH; insol. Me_2CO. Mp 243°.

▷ Oxidiser, highly toxic.

Monohydrate: [7787-38-4].
$BaH_2N_2O_5$ M 247.3
Cryst. from aq. solns. of $Ba(NO_2)_2$. Commercially available. Reagent for converting metal sulfates to metal nitrites; piezoelectric and pyroelectric. Pale yellow hexagonal cryst.; dec. on heating with H_2O loss (−H_2O at 182°). Undergoes sluggish reversible phase transition at 77°. V. sol. H_2O (63 g per 100 cm^3 at 20°); mod. sol. EtOH; insol. Me_2CO.

▷ Oxidiser, toxic.

Ferrari, A. *et al*, *Period. Mineral.*, 1948, **17**, 125 (*cryst struct, monohydrate*)
Patil, K.C. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 155 (*ir, thermal dec*)
Gladkii, V.V. *et al*, *Kristallografiya*, 1967, **12**, 905 (*hydrate, piezoelectric, pyroelectric props*)
Volkov, A.F. *et al*, *Fiz. Tverd. Tela (Leningrad)*, 1975, **6**, 44; *CA*, 1977, **87**, 60359 (*hydrate, Ba-137 nqr*)
Drozhdin, S.N. *et al*, *Izv. Akad. Nauk SSSR, Ser. Fiz.*, 1975, **39**, 990 (*pyroelectric props*)
Bhalla, A.S. *et al*, *Ferroelectrics*, 1981, **38**, 935 (*hydrate, pyroelectric props*)
Gallagher, P.K. *et al*, *J. Chem. Phys.*, 1981, **75**, 1903 (*hydrate, thermal props*)
Wood, D.L., *J. Chem. Phys.*, 1981, **75**, 4809 (*ir, props*)
Warrington, S.B. *et al*, *Proc. Eur. Symp. Therm. Anal., 2nd*, 1981, 315; *CA*, 1982, **96**, 87997 (*thermal props*)
Kvick, A. *et al*, *J. Chem. Phys.*, 1982, **76**, 5508 (*hydrate, cryst struct, nd*)
Lambda, O.P. *et al*, *J. Phys. Chem. Solids*, 1983, **44**, 445 (*hydrate, ir, raman*)
Eriksson, A. *et al*, *J. Mol. Struct.*, 1986, **140**, 19 (*hydrate, ir, raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 336D.

IC-001337

BaN_2O_6

Barium nitrate ($Ba(NO_3)_2$)

Nitric acid, barium salt, 8CI. Nitrobarite

[10022-31-8]

$Ba(NO_3)_2$

M 261.3
Rare as mineral (nitrobarite). Isotypic with $Pb(NO_3)_2$. Prepd. by slow neutralisation of $Ba(OH)_2$ by aq. HNO_3. Commercially available. Component of fireworks giving green colouration to flames. Single cryst. have potential use as active media for solid-body induced Raman scattering transformers. Colourless cubic cryst. Dec. on heating with evolution of NO_2 and O_2 and formation of BaO. V. sol. H_2O (8.7 g per 100 cm^3 at 20°; 34.2 g per 100 cm^3 at 100°); insol. EtOH. Mp 592°. ΔH_f° −992 kJ mol^{-1}, ΔG_f° −797 kJ mol^{-1}, S° 214 J K^{-1} mol^{-1}.

▷ Oxidiser, highly toxic. CQ9625000.

Swanson, H.E. *et al*, *J. Res. Natl. Bur. Stand. (U.S.)*, 1951, **46**, 318 (*cryst struct*)
Chusan, D.E. *et al*, *Appl. Spectrosc.*, 1970, **24**, 283 (*ir, detn*)
Brooker, M.H. *et al*, *J. Chem. Phys.*, 1970, **53**, 1083 (*ir, raman*)
Korshunov, A.V. *et al*, *Zh. Prikl. Spektrosk.*, 1973, **18**, 925 (*raman*)
Muyskens, D.J. *et al*, *Encycl. Chem. Process. Des.*, 1977, **4**, 50 (*rev, ind bibl*)
Ger. Pat., 2 629 949, (1977); *CA*, **86**, 192080 (*use, pyrotechnics*)
Bortkevich, A.V. *et al*, *Zh. Prikl. Spektrosk.*, 1982, **37**, 332 (*uses*)
Chiranjivi, T. *et al*, *Bull. Electrochem.*, 1985, **1**, 585 (*transport props*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 345.

BaN_6

IC-001338

Barium azide ($Ba(N_3)_2$), 8CI

[18810-58-7]

$Ba(N_3)_2$

M 221.3
Prepd. by slow neutralisation of $BaCO_3$ with aq. HN_3 obt. by passing aq. NaN_3 soln. through an ion exchange column. Cryst. from H_2O as the monohydrate. Cryst. in anhydrous form from aq. Me_2CO, aq. MeOH or aq. EtOH. Commercially available in aq. soln. (15%). Monoclinic cryst., dec. on heating with loss of N_2 at about 120°. V. sol. H_2O (17 g per 100 cm^3 at 17°); spar. sol. EtOH (1.7×10^{-2} g per 100 cm^3 at 16°); insol. Et_2O.

▷ Explosive. Toxic. CQ8510000.

Torkar, K. *et al*, *Monatsh. Chem.*, 1965, **96**, 932 (*synth, cryst struct*)
Marinkas, P.L., *Nature (London)*, 1966, **211**, 1288 (*synth*)
Verneker, V.R.P. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 327 (*synth*)
Choi, C.S., *Acta Crystallogr., Sect. B*, 1969, **25**, 2638 (*cryst struct*)
Tompkins, F.C., *Proc. Robert A. Welch Found. Conf. Chem. Res.*, 1970, **14**, 203 (*rev, thermal dec*)
Verneker, V.R.P. *et al*, *J. Phys. Chem.*, 1978, **82**, 735 (*thermal dec*)
Zeman, S. *et al*, *Thermochim. Acta*, 1984, **80**, 137 (*thermal dec*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 340.

$BaNaNdO_9Si_3$

IC-001339

Barium neodymium sodium silicate ($BaNdNa(Si_3O_9)$)

[90936-19-9]

$NaBaNd[Si_3O_9]$

M 532.8
Synthetic, unbranched, monocyclosilicate (three SiO_4 tetrahedra condensed into $[Si_3O_9]$ rings). Synth. hydrothermally from $Na_2O/BaO/Nd_2O_3/SiO_2/H_2O$ system. Cryst.

Malinovskii, Yu.A. *et al*, *Sov. Phys.-Dokl. (Engl. Transl.)*, 1984, **29**, 166 (*cryst struct*)

$BaNa_2O_6Si_2$

IC-001340

Barium sodium silicate ($BaNa_2(Si_2O_6)$)

[51118-20-8]

$Na_2Ba[Si_2O_6]$

M 335.4
Struct. comprises infinite SiO_3 chains linked through 5- and 6- coord. Na and 8-coord. Ba. Phase in the $Na_2O/BaO/SiO_2$ system. Strongly piezoelectric. Monoclinic cryst. stable to 2*M* NaOH and H_2O, leached by 2*M* HCl. Mp 895° (incongr.). Weakly birefringent.

Gunawardane, R.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2397 (*cryst struct*)
Gunawardane, R.P. *et al*, *Trans. J. Brit. Ceram. Soc.*, 1973, **72**, 299 (*synth, struct, props*)
Gunawardane, R.P. *et al*, *J. Am. Ceram. Soc.*, 1974, **57**, 201 (*phases*)
Krol, D.M. *et al*, *J. Phys. Colloq.*, 1982, **C9**, 347 (*raman*)

$BaNa_2O_{14}Si_4Ti_2$ IC-001341

Batisite, 9CI

[12419-32-8]

$Na_2BaTi_2[Si_4O_{12}]O_2$ or $Na_2BaTi_2(Si_2O_7)_2$

M 615.4

Mineral. A single chain silicate. Occurs in the Inaglina nepheline syenite pegmatite, Central Aldan, USSR. Dark brown, elongated orthorhombic cryst. or rosy powder. Mp 1005°.

[87434-85-3]

Kravchenko, S.M. *et al*, *Am. Mineral.*, 1960, **45**, 908 (*mineral*)
Nikitin, A.V. *et al*, *Dokl. Akad. Nauk SSSR*, 1962, **146**, 1401; *CA*, **58**, 5115b (*cryst struct*)

[BaNbS] IC-001342

Barium niobium sulfides

Barium niobium sulfide ($Ba_4Nb_2S_{10}$) [95567-78-5]

(Dithio)octathioxodiniobate(8−) barium salt (1:4)

$Ba_4Nb_2S_{10}$ M 1055.7

Idealised composition. The actual composition is close to $Ba_3NbS_4(S_2)_1$. The layer struct. of BaS_3 layers in sequence CBDBABDBCBCDCACDCB (D is a disordered layer); Nb is between the layers in groups of 2 and of 3 face shared octahedra they being separated by the D layers. Synth. by heating 6BaS + 3Nb + 7S to 1000° in an evacuated graphite ampoule. Black solid.

Barium niobium sulfide ($Ba_4Nb_2S_9$) [85341-12-4]

Nonathioxodiniobate(V)(8−) barium salt (1:4), 11CI. Nonathioxodiniobate(8−) tetrabarium salt, 10CI

$Ba_4Nb_2S_9$ M 1023.7

The struct. comprises hexagonal BaS_3 layers in sequence DABABDBCBCDCACAD. The Nb are in sets of 3 face shared octahedra with D layers above and below (D is a disordered layer). The outer Nb are displaced towards the central Nb. Synth. from 4BaS + 2Nb + 5S at 1000°. Black solid.

Swinnea, J.S. *et al*, *J. Solid State Chem.*, 1985, **56**, 249 (*synth, cryst structs*)

$BaNiO_3$ IC-001343

Barium nickel(*IV*) oxide ($BaNiO_3$)

Barium nickelate

[11081-91-7]

$BaNiO_3$

M 244.0

Structure contains NiO_6 octahedra sharing faces to give $[NiO_3]$ chains. Grey-green solid. Mp 1160°. Sr analogue isostructural.

Lander, J.J., *J. Am. Chem. Soc.*, 1951, **73**, 2452 (*synth*)
Takeda, Y. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 2464 (*cryst struct*)

BaO IC-001344

Barium oxide (BaO), 8CI

[1304-28-5]

BaO

M 153.3

NaCl struct. Prepd. by thermal dec. of $Ba(NO_3)_2$, $Ba(OH)_2.8H_2O$, $BaCO_3$ or BaO_2. Manuf. by heating $BaSO_4$ by d.c. concurrently with plasma gas to 2000-3000 K; the product condenses to a fine powder with particle size of 1-50 μm. Commercially available. An effective drying agent. Component of speciality glasses, glazes and ceramics. Doping agent for ZnO varistors. V. pale yellow cubic cryst. Moisture-sensitive. Reacts with $H_2O \rightarrow Ba(OH)_2$. Mod. sol. EtOH; insol. Me_2CO. Mp 1913°. Bp ~2000°. ΔH_f° −548 kJ mol^{-1}; ΔG_f° −520 kJ mol^{-1}; S° 72.1 J K^{-1} mol^{-1}.

▷ Corrosive, toxic. CQ9800000.

Zollweg, R.J., *Phys. Rev.*, 1955, **100**, 671 (*cryst struct*)
Nakhodova, A.P. *et al*, *CA*, 1964, **60**, 15404h (*synth*)
Habashy, G.M. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 57 (*synth*)
U.S.S.R. Pat., 557 999, (1977); *CA*, **87**, 55212 (*manuf*)
Ger. Pat., 149203, (1981); *CA*, 1982, **96**, 106598 (*manuf*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 348 (*thermodynamics*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 337A.

BaO_2 IC-001345

Barium peroxide (BaO_2), 8CI

[1304-29-6]

BaO_2

M 169.3

Prepd. by either action of air or O_2 on BaO at 500-600° or by thermal dec. of $BaCO_3$, $Ba(C_2O_4).0.5H_2O$ or $Ba(OH)_2.8H_2O$ in air. Alternatively produced by neutralisation of aq. $Ba(OH)_2$ solns. with H_2O_2. Conveniently prepd. by oxidation of BaS. Commercially available. Used to produce dil. aq. solns. of H_2O_2 by treatment with dil. H_2SO_4. Powerful oxidising agent. Pale grey powder. Dec. on heating to BaO + O_2. Dissolves in water with formation of H_2O_2. Mp 450°. ΔH_f° −634 kJ mol^{-1}; ΔG_f° −572 kJ mol^{-1}; S° 66 J K^{-1} mol^{-1}.

▷ Oxidiser, corrosive. CR0175000.

Octahydrate: [12230-86-3].

$BaH_{16}O_{10}$ M 313.4

Cryst. from aq. solns of BaO_2. Colourless hexagonal cryst. Dec. on heating with H_2O loss (−$8H_2O$ at 100°). Spar. sol. H_2O; insol. EtOH, Me_2CO, Et_2O.

Bis(hydrogen peroxide) complex: [12230-85-2].

BaH_4O_6 M 237.3

Prepd. by reaction of $Ba(OH)_2$ with 85% H_2O_2 vapour. Dec. on heating with H_2O_2 evolution.

Tsentsipev, A.B. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1967, 2563, 2738 (*deriv, synth, thermal dec*)
Kuprii, V.Z., *Zh. Fiz. Khim.*, 1971, **45**, 179 (*deriv, thermal dec*)
Habashy, G.M. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 57 (*synth*)
Eysel, H.H. *et al*, *Z. Anorg. Allg. Chem.*, 1975, **411**, 97 (*raman*)
Wiedemann, H.G. *et al*, *Proc. Eur. Symp. Therm. Anal., 1st*, 1976, 295; *CA*, 1977, **87**, 59228 (*synth, thermal dec*)
Brunere, V. *et al*, *CA*, 1979, **90**, 129714 (*ir, uv-vis*)
Azuma, Y. *et al*, *Gypsum Lime*, 1979, **162**, 175; *CA*, 1980, **92**, 33171 (*synth, thermal dec*)
Hill, W.D., *J. Chem. Educ.*, 1986, **63**, 441 (*synth*)

BaO_3Pb IC-001346

Barium lead(*IV*) oxide ($BaPbO_3$)

Barium metaplumbate

[12047-25-5]

$BaPbO_3$

M 392.5

Perovskite struct. Synth. from BaO + PbO_2. Ceramic. Orthorhombic cryst.

[39407-21-1]

Hoppe, R. *et al*, *Z. Anorg. Allg. Chem.*, 1957, **293**, 251 (*synth*)
Nitta, T. *et al*, *J. Am. Ceram. Soc.*, 1965, **48**, 642 (*synth, props*)

Riskin, I.V. *et al*, *Zh. Prikl. Khim.* (*Leningrad*), 1970, **43**, 1941; *CA*, **74**, 60821e (*synth, props*)
Thornton, G. *et al*, *Mater. Res. Bull.*, 1976, **11**, 837 (*cryst struct*)
Vidyasagar, K. *et al*, *J. Solid State Chem.*, 1985, **58**, 29 (*synth*)
Tsuda, T. *et al*, *J. Phys. Soc. Jpn.*, 1987, **56**, 3032 (*Pb-207 nmr*)

BaO_3Ru IC-001347

Barium ruthenium(*IV*) trioxide ($BaRuO_3$)

Barium ruthenate(IV) ($BaRuO_3$), 10CI

[12009-17-5]

$BaRuO_3$

M 286.3

Exists in three different structural modifications which are formed with increasing pressure. Prep. by heating ruthenium metal with BaO_2 in air at 1000°. Catalyses reduction of $NO \rightarrow N_2$ in automobile emissions. Black cryst. Antiferromagnetic (T_N ~430K); good (but not metallic) electrical conductivity. Single crysts. grown from flux of $BaCl_2$.

9R-hexagonal-form

Form at ambient conditions. A parent struct. type, which contains face shared RuO_6 octahedra; Ru—Ru 255 pm. Unit cell volume 0.0687 nm^3.

4H-hexagonal-form

Obt. on applying pressure of 20 atm. to the ambient form. Once formed, reasonably stable. Unit cell volume 0.0675 nm^3.

6H-hexagonal-form

Obt. on applying pressure of 40-100 atm to the ambient form. Once formed, v. stable (may be heated to 1100° without change). Unit cell volume 0.0659 nm^3.

Donohue, P.C. *et al*, *Inorg. Chem.*, 1965, **4**, 306; 1966, **5**, 335 (*synth, struct*)
Callaghan, A. *et al*, *Inorg. Chem.*, 1966, **5**, 1572 (*magnetism, conductivity*)
Longo, J.M. *et al*, *Mater. Res. Bull.*, 1968, **3**, 687 (*synth, struct*)
Goodenough, J.B. *et al*, *Prep. Methods in Solid State Chem.*, Academic Press, N.Y., 1972, 1 (*structural rev*)
Gibb, T.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1253 (*mössbauer*)
Voorhoeve, R.J.H. *et al*, *Mater. Res. Bull.*, 1974, **9**, 1393 (*catalysis, use*)
Trimble, L.E., *Mater. Res. Bull.*, 1974, **9**, 1405 (*catalysis, use*)
Shelef, M. *et al*, *Platinum Met. Rev.*, 1974, **18**, 2 (*catalysis, use*)
Drillon, M. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1979, **75**, 1193 (*magnetism*)
Seddon, E.A. *et al*, *The Chemistry of Ruthenium*, Elsevier, Amsterdam, 1984, 116.

BaO_3Se IC-001348

Barium selenite ($BaSeO_3$)

Barium selenate(IV). Selenious acid, barium salt (1:1), 8CI

[13718-59-7]

$BaSeO_3$

M 264.2

Prepd. by precipitation from mixed aq. solns. of Na_2SeO_3 and $Ba(ClO_4)_2$. Commercially available. Glass colourant. Oxidises on heating in air to give $BaSeO_4$ at >510°. Thermal dec. results in BaO formation at >1285°. Pract. insol. H_2O (0.017 g per 100 cm^3 at 25°). ΔH_f° −1043.1 kJ mol^{-1}; ΔG_f° −971.9 kJ mol^{-1}; S° 177.0 J K^{-1} mol^{-1}.

▷ Highly toxic.

Selivanova, N.M. *et al*, *Khim. Nauka Promst.*, 1957, **2**, 805; *CA*, 1958, **52**, 10700g.

Leshchinskaya, Z.L. *et al*, *Zh. Neorg. Khim.*, 1963, **8**, 763 (*thermochem data*)
Leshchinskaya, Z.L. *et al*, *Zh. Fiz. Khim.*, 1965, **39**, 2036 (*soly, thermochem data*)
Japan. Pat., 79 124 014, (1979); *CA*, 1980, **92**, 115236 (*use*)
Ebert, M. *et al*, *Collect. Czech. Chem. Commun.*, 1982, **47**, 1923 (*synth, ir*)
Losoi, T. *et al*, *Finn. Chem. Lett.*, 1985, 1 (*synth, ir, thermal dec*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 337C.

BaO_3Si IC-001349

Barium silicate ($BaSiO_3$)

Barium metasilicate

[13255-26-0]

$BaSiO_3$

M 213.4

Three polymorphic forms are known. Normally obt. as a single chain silicate ($2SiO_4$ units per chain). BaO_8 polyhedra form. corrugated layers in the thermodynamically stable phase above 1350°. Below this temp., struct. (not the thermodynamic product.) contains cyclic anions instead of the silicate chain. Prepd. from $BaCl_2$ and Na_2SiO_3. Cryst. Insol. H_2O. Mp 1604°. $BaSiO_3$ below 1350°.

Schwarz, R. *et al*, *Ber.*, 1927, **60**, 2263 (*synth*)
Hoehne, E. *et al*, *Acta Crystallogr.*, 1961, **14**, 1298 (*cryst struct, hydrate*)
Lazarev, A.N. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1961, **140**, 811; *CA*, **56**, 8107e (*struct*)
Kruger, G. *et al*, *Z. Anorg. Allg. Chem.*, 1965, **340**, 277 (*synth*)
Grebenshchikov, R.G. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 1620; *CA*, **69**, 90769j (*polymorphs*)
Grosse, H.P. *et al*, *Cryst. Struct. Commun.*, 1974, **3**, 603 (*cryst struct*)
Yamaguchi, O. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 445 (*synth*)
Krol, D.M. *et al*, *J. Phys. Colloq. C*, 1982, **9**, 347 (*raman*)
Timken, H.K.C. *et al*, *J. Phys. Chem.*, 1987, **91**, 1054 (*O-17 nmr*)

BaO_3Sn IC-001350

Barium tin oxide ($BaSnO_3$), 8CI

Barium stannate (1:1), 10CI. Barium metastannate

[12009-18-6]

$BaSnO_3$

M 304.0

Perovskite struct. Prepd. by high temp. reaction of equimolar mixts. of $BaCO_3$ and SnO_2. High purity products are obt. by thermal dec. of $BaSn(C_2O_4)_2.0.5H_2O$. Crude products can be purified by treatment with dilute acids. Used as calibration standard in Mössbauer spectroscopy. Readily forms solid solns. with $BaTiO_3$ and similar ternary oxides. These materials are much used as dielectric ceramics in electrical capacitors. Heavy white powder or pale grey cubic cryst. Spar. sol. H_2O; sol. HNO_3.

▷ Toxic.

Megaw, H.D., *Proc. Phys. Soc., London*, 1946, **58**, 133 (*cryst struct*)
Poix, P., *Bull. Soc. Fr. Ceram.*, 1966, **72**, 3 (*cryst struct*)
Nakamura, T. *et al*, *Jpn. J. Appl. Phys.*, 1966, **5**, 1191 (*dielectric props of solid solns with $BaTiO_3$*)
Dupuis, T. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1967, **264**, 1019 (*ir*)
Gallagher, P.K. *et al*, *Therm. Anal., Proc. Int. Conf., 3rd*, 1971, 1971, **2**, 623; *CA*, 1973, **78**, 131560 (*synth, mössbauer*)
Hannaford, P. *et al*, *J. Phys. C*, 1973, **6**, 2223 (*mössbauer*)
Crecelius, G., *J. Phys. Soc. Jpn.*, 1973, **34**, 579 (*mössbauer*)

Japan. Pat., 80 19 006, (1980); *CA*, **93**, 196585 (*purifn*)
Japan. Pat., 58 209 806, (1983); *CA*, **100**, 165248 (*use*)
Japan. Pat., 59 121 164, (1984); *CA*, **101**, 215429 (*use*)

IC-001351

BaO_3Ti

Barium titanium oxide ($BaTiO_3$)

Barium titanate ($BaTiO_3$), 10CI. Barium metatitanate

[12047-27-7]

$BaTiO_3$

M 233.2

Has the cubic perovskite structure above 120°; below 120° it transforms successively to 3 ferroelectric phases. Prepd. by heating an intimate mixt. of TiO_2 and $BaCO_3$ at ~1300°. Used in electronic devices, e.g. dielectric amplifiers, in computer elements, in memory devices and in ferroelectric ceramics. Light grey-buff powder. Ferroelectric. Insol. H_2O. Mp 1625°.

Clabough, W.S. *et al*, *J. Res. Natl. Bur. Stand. (U.S.)*, 1956, **56**, 289 (*synth*)
Jona, F. *et al*, *Intern. Series of Monographs on Solid State Physics. Vol. I Ferroelectric Crystals*, Pergamon, Oxford, 1962, 108 (*ferroelectricity, rev*)
Inorg. Synth., 1973, **14**, 142 (*synth, cryst*)
Subbarao, E.C., *Solid State Chem.*, 1974, 635 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **3**, 479; **10**, 9
Courtel, M. *et al*, *Oxid. Met.*, 1979, **13**, 77 (*synth*)
Kirby, K.W., *Mater. Res. Bull.*, 1980, **23**, 881 (*synth*)
Diaz-Guemes, M.J. *et al*, *Spectrochim. Acta, Part A*, 1989, **45**, 5 (*ir*)

IC-001352

BaO_4Re

Barium rhenate(*VI*) ($BaReO_4$)

Barium rhenium oxide ($BaReO_4$)

[22655-63-6]

$BaReO_4$

M 387.5

Has distorted Scheelite struct. Synth. from ReO_3 and BaO at 1200° and 6.5 x 10^8 atm. Black powder. Dec. at 680° in air.

Shaplygin, I.S. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 1222 (*synth, props, struct*)

IC-001353

BaO_4S

Barium sulfate ($BaSO_4$)

Sulfuric acid, barium salt (1:1), 8CI. Barosperse. Barotrast. Exophotrast. Oratrast. Trasod. Numerous proprietary names

[7727-43-7]

$BaSO_4$

M 233.3

Manuf. from barite by classical extraction methods. Commercially available. Used for gravimetric determination of barium. Used extensively as an inert filler material. Diagnostic aid (radiopaque medium). White orthorhombic cryst. Undergoes orthorhombic to monoclinic phase transition at 1149°. Spar. sol. H_2O (0.000246 g per 100 cm^3 at 25°; 0.000413 g per 100 cm^3 at 100°). Mp 1580°. ΔH_f° −1473 kJ mol^{-1}; ΔG_f° −1362 kJ mol^{-1}; S° 132 J K^{-1} mol^{-1}.

▷ Toxic. CR0600000

Mineral form [13462-86-7]
Barite. Baryte

Widespread occurrence in hydrothermal deposits. Colourless to greyish, yellowish to deep brown, bluish, greenish, reddish, tabular cryst.

Swanson, H.E. *et al*, *Natl. Bur. Std. Circ. (U.S.)*, 1954, **3**, 65 (*cryst struct*)
Sibbing, E., *Ind. Miner. (London)*, 1976, **101**, 33 (*rev, bibl*)
Dawson, P. *et al*, *Spectrochim. Acta, Part A*, 1977, **33**, 83 (*ir, raman*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 1552.
Volz, F.E., *Appl. Opt.*, 1983, **22**, 1842 (*ir, reflectance*)
Bently, A. *et al*, *Pharm. J.*, 1987, **1**, 138 (*pharmacol*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 337D (*haz*)

IC-001354

BaO_4Se

Barium selenate(*VI*) ($BaSeO_4$)

Selenic acid, barium salt (1:1), 8CI

[7787-41-9]

$BaSeO_4$

M 280.2

Isostructural with $BaSO_4$. Prepd. by addition of aq. $BaCl_2$ to a soln. of SeO_3 in aq. HCl. Sustained release selenium supplement for livestock, esp. sheep. White orthorhombic cryst. Dec. on heating with O_2 loss and formation of $BaSeO_3$. Spar. sol. H_2O (0.018 g per 100 cm^3 at 25°; 0.138 g per 100 cm^3 at 100°). ΔH_f° −1168kJ mol^{-1}; S° 96.5 J K^{-1} mol^{-1}.

▷ Highly toxic.

Selivanova, N.M. *et al*, *Khim. Nauka Promst.*, 1957, **2**, 805; *CA*, 1958, **52**, 10700g (*thermal dec*)
Selivanova, N.M. *et al*, *Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1959, 187; *CA*, **53**, 21121d (*thermochem data*)
Pistorius, C.W.F.T. *et al*, *Z. Kristallogr.*, 1962, **117**, 259 (*cryst struct*)
Mochalov, K.N. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1966, **167**, 361 (*synth*)
Muller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **391**, 38 (*pe*)
Scheuermann, W. *et al*, *J. Raman Spectrosc.*, 1973, **1**, 605 (*ir, raman*)
Cawley, G.D. *et al*, *Vet. Rec.*, 1984, **114**, 565 (*uses*)

IC-001355

BaO_4U

Barium uranate(*VI*) ($BaUO_4$)

Barium uranium(VI) oxide ($BaUO_4$)

[13718-61-1]

$BaUO_4$

M 439.3

6-Coord. at U: U—O 188.7 (x2), 218 (x2), 221 (x2) pm. Orange (yellow) solid. Similar structs. found for $PbUO_4$, $BaHfO_4$, β-$SrUO_4$.

Loopstra, B.O. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 787 (*cryst struct*)
Reis, A.H., *J. Inorg. Nucl. Chem.*, 1976, **38**, 1481 (*cryst struct*)
Allen, G.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 315 (*synth, ir, raman*)
Allen, G.C. *et al*, *Transition Met. Chem.*, 1981, **6**, 355 (*uv-vis*)

IC-001356

BaO_4W

Barium tungstate(*VI*) ($BaWO_4$)

[7787-42-0]

$BaWO_4$

M 385.1

Scheelite ($CaWO_4$) struct. Synth. by several methods e.g. from alkali metal tungstate solns. by metathetical reactions; fusion of WO_3 with metal oxide or carbonate. Used in oxide cathodes. Insol. H_2O, org. solvs. Mp 1490°.

Rieck, G.D., *Tungsten and its Compounds*, Pergamon, Oxford, 1967, 103.

BaO_6P_2

IC-001357

Barium metaphosphate, 9CI, 8CI

[13762-83-9]

$[Ba(PO_3)_2]_x$

M 295.2

Known in amorphous, cryst. and vitreous forms. Synth. from $BaCO_3$ + $(NH_4)_2HPO_4$ at 465-500°; by heating $Ba(H_2PO_4)_2$ at >500°. Both methods yield amorphous salt which cryst. at ≥600°. Component of optical glasses. Mp 875°.

α-form

The existence of this phase has been questioned. Stated to be formed from β-form at 785°, and from $BaCO_3$ + Na_2CO_3 + H_3PO_4 at 380°. Slender plates or lozenge-shaped cryst.

β-form

Orthorhombic. P—O 143-165 pm and OPO 95-122°. Synth. from $BaCO_3$ + H_3PO_4 at 350°. Colourless prisms with pyramidal tetragonal ends. At 785°, reversibly yields the α-form.

γ-form

Monoclinic. Chains formed of 4 PO_4 tetrahedra sharing corners with P—O 147-163 pm, OPO 97-120°. $Ba^{2\oplus}$ ions are octa coordinated by oxygens in an irregular dodecahedron with Ba—O 269-306 pm. Synth. by the rapid dehydration of $Ba(H_2PO_4)_2$ at 500-600°.

Klement, R. *et al*, *Chem. Ber.*, 1960, **93**, 156 (*synth*)
Grenier, J.C. *et al*, *Bull. Soc. Fr. Minéral. Cristallogr.*, 1967, **90**, 24; 1975, **98**, 107 (*synth, cryst struct*)
Muldagaliev, Kh.Kh. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1973, **9**, 646; *Inorg. Materials (Engl. Transl.)*, 1973, **9**, 583 (*ir, raman, struct*)
Nikolina, G.P. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, **10**, 857; 1978, **14**, 1886; *Inorg. Materials (Engl. Transl.)*, 1974, **10**, 734; 1978, **14**, 1460 (*synth, ir, props*)
Exarhos, G.J. *et al*, *J. Chem. Phys.*, 1974, **60**, 4145 (*ir*)
Kuzmenkov, M.I. *et al*, *Zh. Neorg. Khim.*, 1974, **19**, 1621; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 881 (*synth, reactions*)
Cong-Boyat, J. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 2689 (*cryst struct*)
Miroshnichenko, O.Ya. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2936; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1631 (*ir*)
Pinkies, A. *et al*, *Cryst. Res. Technol.*, 1983, **18**, 595 (*synth*)
Lavrov, A.V. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1984, **20**, 271; *Inorg. Materials (Engl. Transl.)*, 1984, **20**, 226 (*synth, ir*)

BaO_6U_2

IC-001358

Barium uranate(*VI*) (BaU_2O_7)

[10380-31-1]

BaU_2O_7

M 725.3

6-Coord. at U. Contains two short U—O bonds (corresponding to $UO_2^{2\oplus}$) and four longer U—O bonds. Yellow microcryst.

Allpress, J.G., *J. Inorg. Nucl. Chem.*, 1965, **27**, 1521 (*synth, cryst struct*)

Allen, G.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 315 (*synth, ir, raman*)
Allen, G.C. *et al*, *Transition Met. Chem.*, 1981, **6**, 355 (*uv-vis*)

BaO_8Tc_2

IC-001359

Barium pertechnetate ($Ba(TcO_4)_2$)

Barium technetate (1−) (1:2). Barium technetium oxide ($BaTc_2O_8$)

$Ba(TcO_4)_2$

M 627.2

Synth. by evaporating a soln. of $BaCO_3$ in $HTcO_4$. Enthalpy of soln. 38 kJ mol^{-1}. White solid, stable to 700°; isotypic with monoclinic $Ba(ReO_4)_2$. Heating with BaO gives $Ba_5(TcO_6)_2$. Mod. sol. H_2O.

Keller, C. *et al*, *Radiochim. Acta*, 1966, **5**, 87 (*synth, struct*)
Majundar, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 33 (*soln props*)

BaO_9Si_3Ti

IC-001360

Benitoite

Barium titanium silicate ($BaTi(Si_3O_9)$)

[15491-35-7]

$BaTi[Si_3O_9]$

M 413.4

Unbranched monocyclosilicate (3 SiO_4 tetrahedra per unit). Mineral, occurs in California, Texas and Belgium. Gemstone. Rhombohedral, blue, purple or colourless cryst.

Fischer, K., *Z. Kristallogr.*, 1969, **129**, 222 (*cryst struct*)
Magi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

$BaO_{12}P_2U_2$

IC-001361

Barium uranyl phosphate ($Ba(UO_2)_2(PO_4)_2$)

Uranocircite. Meta-uranocircite

[59295-99-7]

$Ba(UO_2)_2(PO_4)_2$

M 867.3

Member of autinite group. Mineral, occurs in Germany, the USA. Yellow cryst. + $12H_2O$. Obt. as 6-$8H_2O$ (meta-uranocircite) and 10-12 H_2O (uranocircite).

Ross, M. *et al*, *Am. Mineral.*, 1965, **50**, 1
Weigel, F. *et al*, *J. Less-Common Met.*, 1976, **44**, 99
Gmelin Handbook Inorg. Chem., Syst. No. 55, Suppl. Vol., 1981, **C14**, 95 (*res, bibl*)
Cejka, J. *et al*, *Phys. Chem. Miner.*, 1984, **11**, 173 (*ir*)
Weigel, F., *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, **1**, 365, 371 (*props*)

BaS

IC-001362

Barium sulfide (BaS), 8CI

[21109-95-5]

BaS

M 169.3

NaCl struct. Manuf. from $BaSO_4$ by reduction with graphite, coke or natural gas. Prepd. by reduction of $BaSO_4$ with H_2 at 950° for 1 h. Readily converted to BaO_2 by reaction with O_2. Colourless cubic cryst. Moisture-sensitive. Hydrol. in H_2O with formation of $Ba(OH)_2$ and H_2S. Mp 1200°. ΔH_f° −464 kJ mol^{-1}; ΔG_f° −459 kJ mol^{-1}; S° 78 J K^{-1} mol^{-1}.

▷ Toxic.

Günter, O.J. *et al*, *Z. Kristallogr.*, 1958, **107**, 357 (*cryst struct*)
Muyskens, D.J. *et al*, *Encycl. Chem. Process. Des.*, 1977, **4**, 50 (*uses, bibl*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 352 (*thermochem data*)
Ecker, H. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2140 (*S-33 nmr*)
Hill, W.D., *J. Chem. Educ.*, 1986, **63**, 441 (*reactions*)

IC-001363

BaS_2Sn

Barium tin sulfide ($BaSnS_2$)

[50924-36-2]

$BaSnS_2$

M 320.1
Composite BaS/SnS in distorted NaCl structure. Ba is 6-coordinate (distorted O_h). Sn bonded to 3S atoms only. Cations are ordered so that Ba layers alternate with Sn layers. Sn considered distorted T_d with lone pair at one vertex. Synth. from BaS and SnS fired at 750° for 2 weeks. Yellow-orange cryst. or red-orange powder with slight metallic lustre.

Hervieu, M. *et al*, *Bull. Soc. Chim. Fr.*, 1967, **6**, 2189 (*synth, struct*)
Iglesias, J.E. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 1480 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 46, 1975, **C3**, 201 (*rev, bibl*)

IC-001364

BaS_3

Barium sulfide (BaS_3), 9CI

Barium trisulfide

[12231-01-5]

$Ba(S_3)$

M 233.5
Original molecular struct. correct although cryst. parameters subsequently shown to be incorrect. Prepared by passage of $N_2/H_2S/H_2O$ (50:48:2) gas mixture through a bed of $BaSO_3$ at 470°, or by heating a mix. of $BaCS_3$ and S at 550°. Lemon yellow tetragonal cryst. Mp 554°. Dec. at 600° → S + BaS_2.

Miller, W.S. *et al*, *Z. Kristallogr.*, 1936, **94**, 439 (*cryst struct*)
Marecek, J. *et al*, *Collect. Czech. Chem. Commun.*, 1968, **33**, 4382 (*synth*)
Phillipot, E. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **266**, 1499 (*synth*)
von Schnering, H.G. *et al*, *Naturwissenschaften*, 1974, **61**, 272 (*synth, thermal dec, cryst struct*)
Yamaoka, S. *et al*, *Inorg. Chem.*, 1975, **14**, 129 (*cryst struct*)
Janz, G.J. *et al*, *Inorg. Chem.*, 1976, **15**, 1751 (*raman*)

IC-001365

BaS_3Ta

Barium tantalum sulfide ($BaTaS_3$), 8CI

Barium trisulfidotantalate(IV)

[12009-32-4]

$BaTaS_3$

M 414.4
Hcp has $CsNiCl_3$ struct. *Cf.* Tantalum thallium sulfide ($TaTlS_4$), IC-021900 which contains discrete $TaS_4^{3\ominus}$ ions. Synth. by heating BaS, Ta and S at 600° for 2 weeks then 1000° for 1 week. Semiconductor, activation energy 0.01-0.06eV.

Gardner, R.A. *et al*, *Inorg. Chem.*, 1969, **8**, 2784 (*synth, cryst struct, props*)

IC-001366

$Ba_2CaCu_2O_7Tl$

Barium calcium copper thallium(*III*) oxide ($Ba_2CaCu_2TlO_7$)

Dibarium calcium thallium(III) *dicopper heptoxide*

[117105-30-3]

$(TlO)(BaO)_2Ca(CuO_2)_2$

M 758.2
Tetragonal struct. containing monolayer Tl—O sheets and CuO_2 bilayers. Synth. by solid state reaction of Tl_2O_3, CuO, BaO_2, CuO in sealed quartz tubes at 880°. Superconducting trans. temp. 65-85K. Black.

▷ Toxic.

Hervieu, M. *et al*, *J. Solid State Chem.*, 1988, **75**, 212 (*synth, props*)
Ganguli, A.K. *et al*, *Mod. Phys. Lett. B*, 1988, **2**, 1169 (*synth*)
Parkin, S.S.P. *et al*, *Phys. Rev. Lett.*, 1988, **61**, 750 (*struct, synth*)

IC-001367

$Ba_2CaCu_2O_8Tl_2$

Barium calcium copper thallium(*III*) oxide ($Ba_2CaCu_2Tl_2O_8$)

Dibarium calcium dithallium(III) *dicopper octaoxide*

[115833-27-7]

$(Tl_2O_2)(BaO)_2Ca(CuO_2)_2$

M 978.5
Tetragonal struct. contains Tl-O and Cu-O bilayers. Synth. by solid state reaction of Tl_2O_3, CaO and $BaCu_3O_4$ at 880-910° in O_2. High temp. superconductor; transition temp. 110K. Black rod-shaped cryst.

▷ Toxic.

Maignan, A. *et al*, *Mod. Phys. Lett. B*, 1988, **2**, 681 (*struct, prop, synth*)
Subramanian, M.A. *et al*, *Nature (London)*, 1988, **332**, 420 (*synth, struct*)
Hazen, R.M. *et al*, *Phys. Rev. Lett.*, 1988, **60**, 1657 (*synth, props*)
Wong-Ng, W. *et al*, *Powder Diffr.*, 1988, **3**, 180 (*struct*)

IC-001368

$Ba_2Ca_2Cu_3O_9Tl$

Barium calcium copper thallium(*III*) oxide ($Ba_2Ca_2Cu_3TlO_9$)

Dibarium dicalcium thallium(III) *tricopper nonaoxide*

[116738-74-0]

$(TlO)(BaO)_2Ca_2(CuO_2)_3$

M 893.8
Tetragonal struct., monolayer Tl—O sheets and CuO_2 triple layers. Synth. by solid state reaction of Tl_2O_3, CaO, BaO_2, CuO in sealed quartz tubes at 880°. High temp. superconductor: supercond. transition temp. 100-110K. Black cryst.

▷ Toxic.

Hervieu, M. *et al*, *J. Solid State Chem.*, 1988, **75**, 212 (*synth, props*)
Ganguli, A.K. *et al*, *Mod. Phys. Lett. B*, 1988, **2**, 1169 (*synth*)
Parkin, S.S.P. *et al*, *Phys. Rev. Lett.*, 1988, **61**, 750 (*synth*)

IC-001369

$Ba_2Ca_2Cu_3O_{10}Tl_2$

Barium calcium copper thallium(*III*) oxide ($Ba_2Ca_2Cu_3Tl_2O_{10}$)

Dibarium dicalcium dithallium(III) *tricopper decaoxide. Tl-2223*

[115866-07-4]

$(Tl_2O_2)(BaO)_2Ca_2(CuO_2)_3$

M 1114.2
Tetragonal struct. contains Tl-O bilayers and Cu-O triple layers. Synth. by solid state reaction of Tl_2O_3, CaO, $BaCu_3O_4$ at 880-910° in O_2. High temp. superconductor; superconducting transition temp. 128K. Black.

▷ Toxic.

Hazen, R.M. *et al*, *Phys. Rev. Lett.*, 1988, **60**, 1657 (*synth, struct*)
Hastreiter, G. *et al*, *Solid State Commun.*, 1990, **76**, 1015 (*ir*)
Morosin, B. *et al*, *Physica C: (Amsterdam)*, 1991, **172**, 413 (*cryst struct*)
Edwards, P. *et al*, *Physica C: (Amsterdam)*, 1991, **182**, 110 (*synth, props*)

IC-001370

$Ba_2Cl_2FeH_4O_9Si_2$

Verplanckite

[12178-57-3]

$Ba_2(Mn,Fe,Ti)Si_2O_8(O,OH,Cl,F)_2.3H_2O$

M 607.6
Unbranched monocyclosilicate ($4SiO_4$ tetrahedra per unit). Mineral. Brown-orange cryst.

Kampf, A.R. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 2019 (*cryst struct*)
Povarennykh, A.S., *Mineral. Zh.*, 1979, **1**, 3 (*ir*)

IC-001371

Ba_2CuO_5Tl

Barium copper thallium(*III*) oxide (Ba_2CuTlO_5)

Dibarium thallium(III) *copper pentoxide*

[117728-04-8]

$(TlO)(BaO)_2(CuO_2)$

M 622.5
Tetragonal struct., with Tl—O and CuO_2 sheets. Synth. by solid state reaction of Tl_2O_3, CaO, BaO_2, CuO in sealed quartz tubes at 880°. Black, non-superconducting.

▷ Toxic.

Ganguli, A.K. *et al*, *Mod. Phys. Lett. B*, 1988, **2**, 1169 (*synth*)
Parkin, S.S.P. *et al*, *Phys. Rev. Lett.*, 1988, **61**, 750 (*synth, prop*)

IC-001372

$Ba_2CuO_6Tl_2$

Barium copper thallium(*III*) oxide ($Ba_2CuTl_2O_6$)

Dibarium dithallium(III) *copper hexaoxide*

[115866-06-3]

$Tl_2O_2(BaO)_2(CuO_2)$

M 842.9
Tetragonal struct. contains Tl-O bilayers and Cu-O single layers. Synth. by solid state reaction of Tl_2O_3, $BaCO_3$ and CuO at 880-910° in O_2. Superconducting transition temp. at 80K. Black rod-shaped cryst.

▷ Toxic.

Sheng, Z.Z. *et al*, *Nature (London)*, 1988, **332**, 138 (*synth*)
Sheng, Z.Z. *et al*, *Phys. Rev. Lett.*, 1988, **60**, 937 (*synth, prop*)
Hazen, R.M. *et al*, *Phys. Rev. Lett.*, 1988, **60**, 1657 (*struct*)

IC-001373

$Ba_2Cu_4O_8Y$

Barium copper yttrium oxide ($Ba_2Cu_4YO_8$)

[114104-80-2]

$Ba_2Cu_4YO_8$

M 745.7
High-temp. superconductor with transition temp. 80K.

Marsh, P. *et al*, *Nature (London)*, 1988, **334**, 141 (*cryst struct*)
Marshall, A.F. *et al*, *Phys. Rev. B*, 1988, **37**, 9353 (*formn*)

IC-001374

Ba_2EuO_6Ru

Barium hexaoxoruthenateeuropate (Ba_2RuEuO_6), 10CI

Dibarium europium ruthenium hexaoxide. Barium europium ruthenium oxide (Ba_2EuRuO_6)

[63311-08-0]

Ba_2EuRuO_6

M 623.6
Struct. related to Barium lanthanum ruthenium oxide (Ba_2LaRuO_6), IC-001377. Ferromagnetic solid (T_c 42K). Analogues with Ba replaced by Ca or Sr also known. All contain Ru(V).

Gibb, T.C. *et al*, *J. Solid State Chem.*, 1980, **34**, 279 (*mössbauer*)

IC-001375

$Ba_2H_{12}O_{10}Si_4$

Krauskopfite

[15809-38-8]

$Ba_2H_4[SiO_3]_4.4H_2O$

M 655.0
Unbranched, single chain silicate (4 SiO_4 units per chain). Mineral. White cryst.

Coda, A. *et al*, *Atti R. Accad. Naz. Lincei, Rend. Cl. Sci. Fis., Mat. Nat.*, 1967, **42**, 859 (*cryst struct*)
Coda, A., *Rend. Soc. Ital. Mineral. Petrol.*, 1969, **25**, 195.

IC-001376

Ba_2InO_6Ru

Barium hexaoxoindateruthenate (Ba_2InRuO_6), 10CI

Dibarium indium ruthenium hexaoxide. Barium indium ruthenium oxide (Ba_2InRuO_6)

[77938-15-9]

Ba_2InRuO_6

M 586.5
Contains Ru(V). Possesses the hexagonal $BaTiO_3$ struct. Black hexagonal cryst.

Schaller, H.-U. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **473**, 178 (*synth, powder struct*)

IC-001377

Ba_2LaO_6Ru

Barium lanthanum ruthenium oxide (Ba_2LaRuO_6)

Dibarium lanthanum ruthenium hexaoxide. Barium hexaoxoruthenatelanthanate (Ba_2LaRuO_6), *10CI*

[63311-37-5]

Ba_2LaRuO_6

M 610.6
Ordered, distorted perovskite struct.; monoclinic, with A sites occupied by Ba, and B sites showing ordered arrangement of La and Ru. Prepd. by heating BaO_2 or $BaCO_3$ with Ru or RuO_2 and La_2O_3. Potential catalyst for automobile emission control. Analogues with La replaced by Pr, Nd, Sm, Eu, Gd, Dy, Bi, Y or Yb are also known. All contain Ru(V). Catalyzes the following two reactions: $2NO + 2CO \rightarrow N_2 + 2CO_2$, $2CO + O_2 \rightarrow 2CO_2$.

Donohue, P.C. *et al*, *Mater. Res. Bull.*, 1977, **12**, 519 (*synth, struct, use*)
Bader, H. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **466**, 97 (*synth, struct*)
Battle, P.D., *Mater. Res. Bull.*, 1981, **16**, 397 (*rad*)

Ba_2MnS_3 IC-001378

Barium manganese sulfide (Ba_2MnS_3), 8CI

[12589-60-5]

Ba_2MnS_3

M 425.7
Isostructural with Ba_2MnSe_3 and K_2AgI_3. Synth. from BaS, Mn and S in an evacuated ampoule at 1050°. Orange red cryst.

Brink, C. *et al, Acta Crystallogr.*, 1952, **5**, 433 (*synth, struct*)
Grey, I.E. *et al, Inorg. Chem.*, 1971, **10**, 691 (*struct, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1976, **C6**, 44 (*rev, bibl*)

Ba_2MoO_4 IC-001379

Barium molybdate(*IV*) (Ba_2MoO_4)

Dibarium molybdenum tetroxide

[39416-29-0]

Ba_2MoO_4

M 434.5
Cubic struct. Synth. by reduction of $BaMoO_4$ with H_2. Purple-red solid. Shows metallic behaviour.

Pascal, P., *Nouveau Traité de Chimie Minérale*, Masson, 1976, **5**, 82.

Ba_2MoO_5 IC-001380

Barium molybdate(*VI*) (Ba_2MoO_5)

Barium molybdenum oxide (Ba_2MoO_5)

[54983-00-5]

$Ba_2[MoO_5]$

M 450.5
Quadratic pseudo cubic lattice. Obt. by reaction of $BaMoO_4$ and $BaCO_3$ or Ba_3MoO_6 (solid phase synth.). Mass spectrometric stability of gaseous Ba_2MoO_5 molecules has been studied.

Veksler, S.F. *et al, Zh. Neorg. Khim.*, 1974, **19**, 3224; *CA*, **82**, 67513 (*synth*)
Kudin, L.S. *et al, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1982, **25**, 259; *CA*, **96**, 224188 (*ms*)

Ba_2NbO_6V IC-001381

Barium niobium vanadium oxide (Ba_2NbVO_6), 9CI

[12231-47-9]

Ba_2NbVO_6

M 514.4
Cubic struct. related to perovskite with evidence for ordering of Nb(*V*) and V(*III*) and possibly some pairing of V(*III*). Synth. by heating $NbVO_4$ and $Ba(C_2O_4)$ at 1200° in carefully purified He. Black solid. Paramagnetic: there is evidence for antiferromagnetic coupling of V pairs above 400K. Sr_2TaVO_6 is also known.

Chauvel, C. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1966, **263**, 1536 (*synth, cryst struct*)
Bernier, J.-C. *et al, J. Solid State Chem.*, 1974, **11**, 265 (*synth, cryst struct, magnetism*)

Ba_2O_4Pb IC-001382

Barium lead(*IV*) oxide (Ba_2PbO_4)

Barium orthoplumbate

[12513-70-1]

Ba_2PbO_4

M 545.8
Synth. from $BaPbO_3$ + Li_2O_2. Tetragonal cryst.

Weiss, R. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **248**, 106 (*synth*)
Vidyasagar, K. *et al, J. Solid State Chem.*, 1985, **58**, 29 (*synth*)
Stoll, H. *et al, Z. Anorg. Allg. Chem.*, 1987, **548**, 165 (*synth, cryst struct*)

Ba_2O_4Ru IC-001383

Barium ruthenate (Ba_2RuO_4), 10CI

Dibarium ruthenium tetraoxide. Barium ruthenium oxide (Ba_2RuO_4)

[11130-93-1]

Ba_2RuO_4

M 439.7
K_2NiF_4 struct. Tetragonal cryst.

Goodenough, J.B. *et al, Prep. Methods in Solid State Chem.*, Academic Press, N.Y., 1972, 1 (*synth, cryst struct*)
Prosychev, I.I. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1980, **25**, 489 (*synth*)

Ba_2O_5Re IC-001384

Barium rhenate(*VI*) (Ba_2ReO_5), 12CI

Barium rhenium oxide (Ba_2ReO_5)

[113007-42-4]

Ba_2ReO_5

M 540.8
Isostructural with $K_2VO_2F_3$; contains ReO_4 $O_{2/2}$ octahedra linked by *cis*-bridging O atoms. Interatomic distances: $Re—O_{br}$ 206.9; $Re—O_{term}$ 193.3 pm (av.). Synth. from $Ba_5(ReO_6)_2$ and Re at 800°. Dark grey powder.

Scholder, R. *et al, Angew. Chem., Int. Ed. Engl.*, 1963, **2**, 265.
Cheetham, A.K. *et al, J. Solid State Chem.*, 1987, **71**, 69 (*synth, ir, cryst struct, phases*)

$Ba_2O_5Si_2$ IC-001385

Sanbornite, 9CI

Barium silicate ($Ba_2Si_2O_5$)

[15600-58-5]

$Ba_2[Si_2O_5]$

M 410.8
Mineral. An unbranched single layer silicate. Occurs near Incline, California. Plates.

Rogers, A.F., *Am. Mineral.*, 1932, **17**, 161 (*mineral*)
Douglass, R.M., *Am. Mineral.*, 1958, **43**, 517 (*cryst struct*)
Hesse, K.F. *et al, Z. Kristallogr.*, 1980, **153**, 33 (*cryst struct*)

$Ba_2O_6P_2S_2Se$ IC-001386

Barium bis(phosphonothio) selenide (2:1), 10CI

Barium dithiomonoselenopyrophosphate

[62918-44-9]

$Ba_2[(O)_2P(S)SeP(S)(O)_2]$

M 575.6
Dihydrate: Synth. from $Se(S_2O_2Me)_2$ + Na_3SPO_3 aq. + $Ba(OH)_2$. Needles.

Wagner, H. *et al, Z. Anorg. Allg. Chem.*, 1977, **429**, 270 (*synth, ir*)

Ba_2O_6RhRu IC-001387

Barium hexaoxorhodateruthenate ($BaRhRuO_6$), 10CI

Dibarium rhodium ruthenium hexaoxide. Barium rhodium ruthenium oxide (Ba_2RhRuO_6)

[77908-67-9]

Ba_2RhRuO_6

M 574.6
Contains Ru(*V*). Rhombohedral 9L struct. (*cf.* Barium ruthenium(*IV*) trioxide ($BaRuO_3$), IC-001347). Black cryst.

Schaller, H.-U. *et al, Z. Anorg. Allg. Chem.*, 1981, **473**, 178 (*synth, powder struct*)

Ba_2O_6RuSc IC-001388

Barium hexaoxoruthenatescandate (Ba_2RuScO_6), 10CI

Dibarium ruthenium scandium hexaoxide. Barium ruthenium scandium oxide (Ba_2RuScO_6)

[75036-90-7]

Ba_2ScRuO_6

M 516.6
Contains Ru(*V*). Hexagonal 6L struct. Prepd. as for Barium lanthanum ruthenium oxide (Ba_2LaRuO_6), IC-001377.

Bader, H. *et al, Z. Anorg. Allg. Chem.*, 1980, **466**, 97 (*synth, powder struct*)

$Ba_2O_8Si_3$ IC-001389

Barium silicate ($Ba_4(Si_6O_{16})$)

[14871-82-0]

$Ba_4[Si_6O_{16}]$

M 486.9
Unbranched double chain struct. (3 SiO_4 units long). Cryst.

Hesse, K.-F. *et al, Z. Kristallogr.*, 1980, **153**, 3 (*cryst struct*)

$Ba_2O_{14}Si_4V_2$ IC-001390

Suzukiite, 9CI

[82570-67-0]

$Ba_2V_2[Si_4O_{12}]O_2$

M 712.8
Mineral. A single chain silicate. Occurs at the Mogurazawa mine, Gumma, Japan. Bright green orthorhombic cryst.

Matsubara, S. *et al, Mineral. J.*, 1982, **11**, 15 (*mineral*)

$Ba_2O_{30}P_{10}Zn_3$ IC-001391

Barium zinc metaphosphate ($P_{10}O_{30}^{10\ominus}$) (1:2:3), 11CI

Dibarium trizinc cyclodecaphosphate

[80440-72-8]

$Ba_2Zn_3(P_{10}O_{30})$

M 1260.5
Interconnected $P_{10}O_{30}$ rings, ZrO_4 tetrahedra, ZnO_6 octahedra, and BaO_9 polyhedra. Coordination numbers: Ba 9, Zn 4, 6, and 8. Structure possesses very large channels. Synth. from $BaCO_3$ + ZnO + $(NH_4)_2HPO_4$ or H_3PO_4 at 400-600°. First example of a purified decametaphosphate system.

Bagieu-Beucher, M. *et al, J. Solid State Chem.*, 1981, **40**, 248; 1982, **45**, 159 (*synth, cryst struct*)
Cabello, C.I. *et al, Spectrochim. Acta, Part A*, 1985, **41**, 1359 (*synth, ir, raman*)

Ba_2S_4Sn IC-001392

Barium orthothiostannate

Barium tin sulfide (Ba_2SnS_4)

[12589-70-7]

Ba_2SnS_4

M 521.6
Dimorphic. Tin is tetrahedrally coordinated by S atoms.

Low temp-form
Monoclinic cryst.

High temp-form
Contains two types of distorted tetrahedra. Orthorhombic cryst.

Katuada, M. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 2249 (*synth, mössbauer*)
Jumas, J.C. *et al, J. Solid State Chem.*, 1975, **14**, 319 (*cryst struct*)
Neyrand, M. *et al, Rev. Chim. Minér.*, 1975, **12**, 406 (*ir*)
Greatrex, R. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 500 (*mössbauer, synth*)
Philippot, G. *et al, React. Solids*, [*Proc. Int. Symp.*], *8th*, *1976*, 1977, 535 (*ir, mössbauer, cryst struct*)

$Ba_3CaO_9Ru_2$ IC-001393

Barium calcium ruthenate ($Ba_3CaRu_2O_9$), 10CI

Barium calcium ruthenium oxide ($Ba_3CaRu_2O_9$). Tribarium calcium diruthenium nonaoxide

[61504-95-8]

$Ba_3Ru_2CaO_9$

M 798.1
Contains Ru(*V*). Isostructural with Barium magnesium ruthenium(*V*) oxide ($Ba_3MgRu_2O_9$), IC-001397. Made as for Barium magnesium ruthenium(*V*) oxide ($Ba_3MgRu_2O_9$), IC-001397. Antiferromagnetic solid. Semiconductor (E_g 0.43 eV).

Darriet, J. *et al, J. Solid State Chem.*, 1976, **19**, 213 (*synth, cryst struct*)
Drillon, M., *Solid State Commun.*, 1977, **21**, 425 (*magnetism*)
Fernandez, I. *et al, J. Solid State Chem.*, 1980, **34**, 121 (*mössbauer*)

$Ba_3CdO_9Ru_2$ IC-001394

Barium nonaoxocadmatediruthenate ($Ba_3CdRu_2O_9$), 10CI

Tribarium cadmium diruthenium nonaoxide. Barium cadmium ruthenium oxide ($Ba_3CdRu_2O_9$)

[61504-96-9]

$Ba_3Ru_2CdO_9$

M 870.5
Contains Ru(*V*). Isostructural with Barium magnesium ruthenium(*V*) oxide ($Ba_3MgRu_2O_9$), IC-001397. Made as for Barium magnesium ruthenium(*V*) oxide ($Ba_3MgRu_2O_9$), IC-001397. Antiferromagnetic solid.

Darriet, J. *et al, J. Solid State Chem.*, 1976, **19**, 213 (*synth, cryst struct*)
Fernandez, I. *et al, J. Solid State Chem.*, 1980, **34**, 121 (*mössbauer*)

$Ba_3InO_5Ru_2$ IC-001395

Barium nonaoxoindatediruthenate ($Ba_3InRu_2O_9$), 10CI

Tribarium indium diruthenium nonaoxide. Barium indium ruthenium oxide ($Ba_3InRu_2O_9$)

[77938-16-0]

$Ba_3InRu_2O_9$

M 872.9

Mixed valence compd., containing ruthenium(*V/VI*). Possesses the hexagonal $BaTiO_3$ struct. Black hexagonal cryst.

Schaller, H.-U. *et al, Z. Anorg. Allg. Chem.*, 1981, **473**, 178 (*synth, powder struct*)

Ba_3IrLaO_5Ru IC-001396

Barium nonaoxoiridateruthenatelanthanate (BaIrRuLaO$_5$), 10CI

Tribarium lanthanum iridium ruthenium nonaoxide. Barium lanthanum iridium ruthenium oxide ($Ba_3LaIrRuO_9$)

[76130-27-3]

$Ba_3LaIrRuO_9$

M 988.1

Possesses the hexagonal $BaTiO_3$ struct. Black hexagonal cryst.

Dürrschmidt, E. *et al, Z. Anorg. Allg. Chem.*, 1980, **470**, 109 (*synth, powder struct*)

Thumm, I. *et al, Z. Anorg. Allg. Chem.*, 1981, **477**, 161 (*synth, powder struct*)

$Ba_3MgO_5Ru_2$ IC-001397

Barium magnesium ruthenium(*V*) oxide ($Ba_3MgRu_2O_9$)

Tribarium magnesium diruthenium nonaoxide

[12231-80-6]

$Ba_3Ru_2MgO_9$

M 782.4

Possesses the hexagonal $BaTiO_3$ struct. The $Ru^{5\oplus}$ ions occupy the face-shared octahedra; the $Ni^{2\oplus}$ ions occupy the corner-shared octahedra. Prepd. by heating a mixture of $BaCO_3$, MgO and Ru in air at 1200°. Antiferromagnetic solid (T_c = 390K). V. low electrical conductivity. Oxidizes aq. HCl to Cl_2. Ru—Ru 263 pm (within face-shared octahedra).

Donohue, P.C. *et al, Inorg. Chem.*, 1966, **5**, 339 (*synth, cryst struct, reactions*)

Callaghan, A. *et al, Inorg. Chem.*, 1966, **5**, 1572 (*magnetism*)

Ba_3MnO_5 IC-001398

Barium manganese oxide (Ba_3MnO_5)

Barium manganate oxide ($Ba_3(MnO_4)O$)

$Ba_3(MnO_4)O$

M 546.9

Contains tetrahedral $[Mn^{VI}O_4]^{2\ominus}$ anion. Isotypic with Cs_3CoCl_5. Synth. from $BaMnO_3$ or $Ba_3(MnO_4)_2$ and $Ba(OH)_2$ (1:1 ratio) under N_2 at 850°.

Scholder, R., *Angew. Chem.*, 1958, **70**, 583.

Mansmann, M., *Z. Anorg. Allg. Chem.*, 1965, **339**, 52 (*cryst struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1975, **C2**, 251 (*rev, bibl*)

Ba_3N_2 IC-001399

Barium nitride (Ba_3N_2), 8CI

[12047-79-9]

Ba_3N_2

M 439.9

Prepd. either by high temp. nitridation of barium or by low temp. reaction of N_3 with solns. of Ba in liq. Na. Also formed as a thermal dec. product of $Ba(N_3)_2$. Reacts with Si_3N_4 to form $BaSiN_2$. Deep purple powder. Extremely moisture-sensitive. Reacts with H_2O with formation of $Ba(OH)_2$ and evolution of NH_3. Dec. on heating to form Ba_3N and N_2. Mp 1000°. ΔH_f° = −363 kJ mol^{-1}; ΔG_f° = −292 kJ mol^{-1}; S° 152 J K^{-1} mol^{-1}.

▷ Toxic.

Torkar, K. *et al, Monatsh. Chem.*, 1967, **98**, 2020 (*synth*)

Orcutt, R.H., *J. Res. Natl. Bur. Stand., Sect. A*, 1970, **74**, 45 (*thermal dec*)

Gaude, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 521 (*synth, reactions*)

Hubberstey, P., *Liq. Alkali Met., Proc. Int. Conf.*, 1973, 15; *CA*, 1974, **81**, 42127 (*synth*)

Linke, K.H. *et al, Z. Anorg. Allg. Chem.*, 1975, **413**, 165 (*synth*)

$Ba_3NaNd_3O_{10}Si_6$ IC-001400

Barium neodymium sodium silicate ($Ba_3Nd_3Na(Si_4O_{13})(Si_2O_7)$)

Barium sodium hexakis[metasilicate(2−)] dioxoneodymate(7−), 9CI

[88705-48-0]

$NaBa_3Nd_3[Si_4O_{13}][Si_2O_7]$

M 1356.1

Phase in the system Na_2O-BaO-Nd_2O_3-SiO_2-H_2O.

Malinovskii, Yu.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1983, **272**, 865; *CA*, **100**, 77671k (*cryst struct*)

Bondareva, O.S. *et al, Kristallografiya*, 1986, **31**, 159 (*formn*)

$Ba_3Nb_6O_{16}Si_4$ IC-001401

Barium niobium oxide silicate ($Ba_3Nb_6O_{12}(Si_2O_7)_2$)

[12449-08-6]

$Ba_3Nb_6[Si_2O_7]_2O_{12}$

M 1497.7

Cryst.

Shannon, J. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 105 (*cryst struct*)

Choisnet, J. *et al, Mater. Res. Bull.*, 1976, **11**, 887 (*synth, cryst struct*)

$Ba_3NiO_5Ru_2$ IC-001402

Barium nickel ruthenium(*V*) oxide ($Ba_3NiRu_2O_9$), 8CI

Tribarium nickel diruthenium nonaoxide. Barium nonaoxonickelatediruthenate ($Ba_3NiRu_2O_9$), 10CI

[12231-84-4]

$Ba_3Ru_2NiO_9$

M 816.8

Possesses the hexagonal $BaTiO_3$ struct. The $Ru^{5\oplus}$ ions occupy the face-shared octahedra; the $Ni^{2\oplus}$ ions occupy the corner-shared octahedra. Prepd. by heating a mixture of $BaCO_3$, $NiCO_3$ and Ru in air at 1100°.

Donohue, P.C. *et al, Inorg. Chem.*, 1966, **5**, 339 (*synth, cryst struct*)

Fernandez, I. *et al, J. Solid State Chem.*, 1980, **34**, 121 (*mössbauer*)

Ba_3O_5Ru IC-001403

Barium ruthenium oxide (Ba_3RuO_5)

Barium ruthenate (Ba_3RuO_5), 10CI. Tribarium ruthenium pentaoxide

[73503-53-4]

Ba_3RuO_5

M 593.0

Rhombic cryst.

Prosychev, I.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 489 (*synth, struct*)

Ba_3O_5Re IC-001404

Barium rhenate(*IV*) (Ba_3ReO_5)

Barium rhenium oxide (Ba_3ReO_5)

Ba_3ReO_5

M 694.1

Ordered distorted perovskite struct. Synth. from $BaCO_3$, $Ba(ReO_4)_2$ and ReO_2 at 800-1000°. Dark grey phase.

Schaider, R. *et al, Angew. Chem., Int. Ed. Engl.*, 1963, **2**, 365 (*synth, props*)

Cheetham, A.K. *et al, J. Solid State Chem.*, 1987, **71**, 61 (*synth, struct, phases*)

$Ba_3O_8P_2$ IC-001405

Barium phosphate ($Ba_3(PO_4)_2$)

Barium phosphate (3:2), 9CI, 8CI. Barium orthophosphate

[13517-08-3]

$Ba_3(PO_4)_2$

M 601.9

Exists in low- and high-temp. stable forms. Also known in vitreous form. Synth. from $BaCO_3$ + MH_2PO_4 at 1100°; $Ba(OH)_2$ + H_3PO_4 at 100°; $BaCl_2$ + KH_2PO_4 aq. When prepared at pH 9-11, product is apatitic in struct. Mp >1620°. With HCl(g) at 700°, gives Barium chloroapatite. Said to be hydrolysable at alk. pH → Barium hydroxyapatite. A phase transition occurs at 715°. *β*-form stable at >1390°; it can be supercooled considerably but cannot be obt. at r.t. by quenching.

Monohydrate: [87896-20-6].

Dehydrates at *ca.* 360°.

Eanes, E.D. *et al, Calcif. Tissue Res.*, 1968, **2**, 38 (*synth, props*)

Mooney, R.W. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 1669 (*synth, ir*)

Hoekstra, A.H. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 2445 (*synth*)

Kreidler, E.R., *J. Electrochem. Soc.*, 1971, **118**, 923 (*props*)

Tarte, P. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 5 (*ir, raman*)

Lazarev, A.N. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1976, **12**, 1240; *Inorg. Materials (Engl. Transl.)*, 1976, **12**, 1032 (*ir, raman*)

Sarawadekar, R.G. *et al, Thermochim. Acta*, 1983, **67**, 333 (*ir, props*)

Lopatin, S.I. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1986, **287**, 380; *Dokl. Chem. (Engl. Transl.)*, 1986, **287**, 249 (*ms*)

Ba_3O_9ReSb IC-001406

Barium antimonate rhenate ($Ba_3(SbO_4)(ReO_5)$)

Nonaoxoantimonaterhenate, barium salt (1:3), 11CI

[81775-31-7]

$Ba_3(ReSbO_9)$

M 863.9

Perovskite related struct. with partially-ordered cationic vacancies. Synth. from BaO, Re_2O_7 + Sb_2O_5 at 600-800° in air. Light yellow cryst.

Kemmler-Sack, S. *et al, Z. Anorg. Allg. Chem.*, 1982, **494**, 173 (*synth, struct, props*)

$Ba_3O_9Re_2$ IC-001407

Barium rhenium oxide ($Ba_3Re_2O_9$)

Barium rhenate(VI) ($Ba_3Re_2O_9$)

[65149-61-3]

$Ba_3Re_2O_9$

M 928.3

Hexagonal struct., sl. Re deficient with two types of octahedral Re sites. Ba 12-coordinate. Re—O 186.1-206.1 pm. Synth. from BaO and ReO_3 at ~6 × 10^3 atm. and 1180°. Cryst. Oxidises slowly in the atm. to $Ba_3(ReO_5)_2$.

Calvo, C. *et al, Inorg. Chem.*, 1978, **19**, 699 (*synth, cryst struct*)

Chamberland, B.L. *et al, J. Solid State Chem.*, 1978, **25**, 79.

Cheetham, A.K. *et al, J. Solid State Chem.*, 1987, **71**, 61.

$Ba_3O_9RhRu_2$ IC-001408

Barium nonaoxorhodatediruthenate ($Ba_3RhRu_2O_9$), 10CI

Tribarium rhodium diruthenium nonaoxide. Barium rhodium ruthenium oxide ($Ba_3RhRu_2O_9$)

[77908-68-0]

$Ba_3RhRu_2O_9$

M 861.0

A mixed valence compd., containing ruthenium (*V/IV*). Rhombohedral 9 L struct. (*cf.* Barium ruthenium(*IV*) trioxide ($BaRuO_3$), IC-001347). Black crystalline solid.

Schaller, H.-U. *et al, Z. Anorg. Allg. Chem.*, 1981, **473**, 178 (*synth, powder struct*)

$Ba_3O_9Ru_2Sm$ IC-001409

Barium nonaoxodiruthenatesamarate ($BaRu_2SmO_9$), 10CI

Barium ruthenium samarium oxide ($Ba_3Ru_2SmO_9$). Tribarium diruthenium samarium nonaoxide

[79103-31-4]

$Ba_3SmRu_2O_9$

M 908.4

Mixed valence compd. containing ruthenium(*V/IV*). Possesses the hexagonal $BaTiO_3$ struct. Black hexagonal cryst.

Dürrschmidt, E. *et al, Z. Anorg. Allg. Chem.*, 1980, **470**, 109 (*synth, powder struct*)

Thumm, I. *et al, Z. Anorg. Allg. Chem.*, 1981, **477**, 161 (*synth, powder struct*)

$Ba_3O_9Ru_2Sr$ IC-001410

Barium strontium ruthenate ($Ba_3SrRu_2O_9$), 10CI

Tribarium strontium diruthenium nonaoxide. Barium ruthenium strontium oxide ($Ba_3Ru_2SrO_9$)

[61505-00-8]

$Ba_3Ru_2SrO_9$

M 845.7

Contains Ru(*V*). Shows a monoclinic distortion from the struct. of Barium magnesium ruthenium(*V*) oxide ($Ba_3MgRu_2O_9$), IC-001397. Made as for Barium magnesium ruthenium(*V*) oxide ($Ba_3MgRu_2O_9$), IC-001397. Antiferromagnetic solid.

Darriet, J. *et al*, *J. Solid State Chem.*, 1976, **19**, 213 (*synth, cryst struct*)
Fernandez, I. *et al*, *J. Solid State Chem.*, 1980, **34**, 121 (*mösshauer*)

IC-001411

$Ba_3O_{10}Re_2$

Barium rhenate(*VII*) ($Ba_3(ReO_5)_2$)

*Tribarium bis(pentaoxorhenate(*VII*)). Barium mesoperrhenate. Barium rhenate ($ReO_5^{3\ominus}$) (3:2), 10CI*

[13598-04-4]

$Ba_3(ReO_5)_2$

M 944.3

Struct. best regarded as a trimeric $Ba_9(ReO_5)_6$ apatite with vacancies. Synth. (i) from $ReO_4^{\ominus}$ aq. and excess of $Ba(OH)_2$ (ii) from $Ba(ReO_4)_2$ and BaO at 600° for 24 h under 8 x 10^3 atm. Yellow cryst. Sol. H_2O with dec. to $ReO_4^{\ominus}$. Loses O_2 on heating to 900°.

Scholder, R. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **334**, 209 (*synth, props*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 3, 1635 (*synth*)
Baud, G. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1605 (*synth, cryst struct, props*)
Baran, E.J. *et al*, *Spectrochim. Acta, Part A*, 1983, **39**, 383 (*synth, ir, raman, struct*)

IC-001412

$Ba_3O_{13}Si_5$

Barium silicate ($Ba_6(Si_{10}O_{26})$)

[12507-96-9]

$Ba_6[Si_{10}O_{26}]$

M 760.4

Unbranched double five-fold chain struct. Cryst. Stable only > 1300°. Below 1300°, dec. to Barium silicate ($Ba_5(Si_8O_{21})$), IC-001425 and $BaSi_2O_5$.

Hesse, K.-F. *et al*, *Z. Kristallogr.*, 1980, **153**, 3 (*cryst struct*)

IC-001413

Ba_3S_5Si

Barium sulfide thiosilicate ($Ba_3S(SiS_4)$)

*Barium silicide sulfide (Ba_3SiS_5). Tribarium tetrathiosilicate(*IV*) sulfide*

[70378-69-7]

$Ba_3S(SiS_4)$

M 600.3

Orthorhombic struct.

Schmitz, D., *Acta Crystallogr., Sect. B*, 1981, **37**, 518 (*cryst struct*)

IC-001414

$Ba_3S_7Sn_2$

Barium tin sulfide ($Ba_3Sn_2S_7$)

Barium thiodistannate

[11071-76-4]

$Ba_3Sn_2S_7$

M 873.8

Monoclinic struct. built up of $Sn_2S_7^{6\ominus}$ anions and $Ba^{2\oplus}$ cations. $Sn_2S_7^{6\ominus}$ results from condensation of $2SnS_4$ tetrahedra with 1 common apex. Coordination of $Ba^{2\oplus}$ relative to S is 8 or 9. Cryst.

Jumas, J.C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1971, **273**, 1356 (*cryst struct*)
Jumas, J.C. *et al*, *Rev. Chim. Minér.*, 1974, **11**, 13 (*cryst struct*)
Greatrex, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 500 (*mösshauer*)
Philippot, E. *et al*, *React. Solids, [Proc. Int. Symp.], 8th*, 1976, 1977, 535 (*cryst struct, ir, mösshauer*)

IC-001415

$Ba_4Ca_2Fe_4O_{34}Si_{12}$

Pellyite

[37187-91-0]

$Ca_2Ba_4(Fe,Mg)_4[Si_{12}O_{34}]$

M 1733.8

Branched, chain silicate. Mineral, occurs as a constituent of skarns at sites in USA. Used in the preparation of ceramics. Colourless or pale yellow translucent cryst. Mp 885-915°.

Meagher, E.P., *Am. Mineral.*, 1976, **61**, 67 (*cryst struct*)
Glasser, F.P. *et al*, *Ceram. Int.*, 1977, **3**, 89 (*synth*)
Pabst, A. *et al*, *Can. Mineral.*, 1984, **22**, 653 (*phys props*)

IC-001416

$Ba_4ClNb_4O_{28}Si_4Ti_4$

Baotite

[12413-85-3]

$Ba_4(Ti,Nb,Fe)_4[Si_4O_{12}]O_{16}Cl$

M 1708.2

Mineral. Unbranched monocyclosilicate (4 SiO_4 tetrahedra per unit). Alternative formulation $Ba_4(Ti,Nb)_8Si_4O_{28}Cl$. Found in Montana and Inner Mongolia. Light brown to black, vitreous cryst.

Nekrasa, Yu.V. *et al*, *Kristallografiya*, 1969, **14**, 602 (*cryst struct*)
Muradyan, L.A. *et al*, *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1977, **22**, 277 (*cryst struct*)
Pavarennykh, A.S., *Mineral. Zh.*, 1981, **3**, 14 (*ir*)

IC-001417

$Ba_4Cu_7O_{15}Y_2$

Barium copper yttrium oxide ($Ba_4Cu_7Y_2O_{15}$)

[124365-83-9]

$Ba_4Cu_7Y_2O_{15}$

M 1411.9

High-temp. superconductor with transition temp. 40K.

Border, P. *et al*, *Nature (London)*, 1988, **334**, 596 (*cryst struct*)

IC-001418

$Ba_4NbO_{12}Ru_3$

Barium dodecaoxotriruthenateniobate ($Ba_4NbRu_3O_{12}$), 10CI

Tetrabarium niobium triruthenium dodecaoxide. Barium niobium ruthenium oxide ($Ba_4NbRu_3O_{12}$). Barium niobium ruthenate ($Ba_4Nb(Ru_3O_{12})$)

[73379-43-8]

$Ba_4Nb[Ru_3O_{12}]$

M 1137.4

Contains the $[Ru_3O_{12}]^{13\ominus}$ unit.

Drillon, M. *et al*, *J. Phys. Chem. Solids*, 1980, **41**, 507.

IC-001419

$Ba_4NiO_{12}Re_2$

Barium nickel rhenate(*VII*) ($Ba_4Ni(ReO_6)_2$)

Barium nickel rhenium oxide ($Ba_4NiRe_2O_{12}$). Barium nickel orthoperrhenate

[13598-05-5]

$Ba_4NiRe_2O_{12}$

M 1172.4

Has hexagonal perovskite struct. with cation vacancies. Ba and Ni cations are replaceable in whole or in part by Sr and Co. Synth. from Re and oxides or carbonates at temps. up to 1000°. Cryst.

Herrman, M. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **476**, 115 (*synth, cryst struct, ir, raman, uv*)

IC-001420

$Ba_4O_{12}Ru_3Ta$

Barium dodecaoxotriruthenatetantalate ($Ba_4Ru_3TaO_{12}$), 10CI

Barium ruthenium tantalum oxide ($Ba_4Ru_3TaO_{12}$). Tetrabarium tantalum triruthenium dodecaoxide. Barium tantalum ruthenate ($Ba_4Ta(Ru_3O_{12})$)

[73379-46-1]

$Ba_4Ta[Ru_3O_{12}]$

M 1225.4

Contains the $[Ru_3O_{12}]^{13\ominus}$ unit.

Drillon, M. *et al*, *J. Phys. Chem. Solids*, 1980, **41**, 507.

IC-001421

$Ba_5BrO_{15}Re_3$

Barium bromide rhenate(*VII*) ($Ba_5Br(ReO_5)_3$)

*Bromopentadecaoxotrirhenate(*VII*), barium salt (1:5), 10CI*

[70992-92-6]

$Ba_5(ReO_5)_3Br$

M 1565.1

Contains distorted square pyramidal $ReO_5^{3\ominus}$ anions with Re—O(av.) 182.5pm. Struct. is related to apatite. Synth. from $BaBr_2$ and Re at 800° in air. Clear yellow needles. Other related Ba salts of $[(ReO_5)_3X]^{10\ominus}$ exist where X = halide, nitrate, $\frac{1}{2}$(carbonate).

Baud, G. *et al*, *Mater. Res. Bull.*, 1979, **14**, 675 (*synth, props, cryst struct*)

IC-001422

$Ba_5Ga_2S_8$

Barium thiogallate ($Ba_5(GaS_4)_2$)

Barium tetrathioxogallate(5−) (2:5), 11CI

[89299-15-0]

$Ba_5(GaS_4)_2$

M 1082.6

Synth. from BaGa, Ba and S at 1150°. Colourless moisture-sensitive prisms (melt).

Eisenmann, B. *et al*, *Z. Naturforsch., B*, 1984, **39**, 27 (*synth, cryst struct*)

IC-001423

$Ba_5NO_{18}Re_3$

Barium nitrate perrhenate ($Ba_5(NO_3)(ReO_5)_3$)

*(Nitrato)pentadecaoxotrirhenate, barium (1:5), 11CI. Pentabarium nitratotris(metaperrhenate(*VII*)). Barium rhenium nitrate oxide ($Ba_5Re_3(NO_3)O_{15}$)*

[85941-78-2]

$Ba_5[(NO_3)(ReO_5)_3]$

M 1547.2

Apatite struct. with distorted square-pyramidal ReO_5 groups, with Re—O at 168.1 to 188.9 pm, average 182.6 pm. Synth. from Re and $Ba(NO_3)_2$ at 600° in air. Clear yellow needles.

Aneas, M. *et al*, *Mater. Chem. Phys.*, 1983, **8**, 119 (*synth, cryst struct*)

IC-001424

$Ba_5O_{12}Re_2$

Barium rhenate(*VII*) ($Ba_5(ReO_6)_2$)

*Barium orthoperrhenate ($Na_5(ReO_6)_2$). Barium hexaoxorhenate(*VII*). Barium rhenium oxide ($Ba_5Re_2O_{12}$)*

[13598-09-9]

$Ba_5(ReO_6)_2$

M 1251.0

Has perovskite-related 24 layer struct. Synth. from $Ba(ReO_4)_2$ and $BaCO_3$ at 1200°. Yellow-orange powder.

Longo, J.M. *et al*, *Inorg. Chem.*, 1965, **4**, 235 (*synth, struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 3, 1636 (*synth*)
Cheetham, A.K. *et al*, *J. Solid State Chem.*, 1987, **71**, 61 (*synth, phases*)

IC-001425

$Ba_5O_{21}Si_8$

Barium silicate ($Ba_5(Si_8O_{21})$)

[11092-02-7]

$Ba_5[Si_8O_{21}]$

M 1247.3

Contains quadruple, oligo-fold, unbranched silicate chain. Cryst.

Planz, J.E. *et al*, *Ber. Dtsch. Keram. Ges.*, 1961, **10**, 440 (*synth, ir*)
Oehlschlegel, G. *et al*, *Glastech. Ber.*, 1971, **44**, 194 (*cryst struct*)
Hesse, K.-F. *et al*, *Z. Kristallogr.*, 1980, **153**, 3 (*cryst struct*)

IC-001426

$Ba_7Ga_4Sb_9$

Barium gallium antimonide ($Ba_7Ga_4Sb_9$)

[102764-89-6]

$Ba_7Ga_4Sb_9$

M 2335.9

Prepd. from the elements. Cryst. with a metallic lustre.

Cordier, G. *et al*, *Z. Anorg. Allg. Chem.*, 1986, **534**, 137 (*synth, cryst struct*)
Alemany, P. *et al*, *Inorg. Chem.*, 1990, **29**, 3070 (*electronic struct*)

IC-001427

$Ba_7K_2O_{40}Si_{16}$

Barium potassium silicate ($Ba_7K_2(Si_4O_{10})_4$)

[82897-69-6]

$K_2Ba_7[Si_4O_{10}]_4$

M 2128.8

Synthetic unbranched single layer silicate. Struct. comprises infinite Si_2O_5 sheets linked by 8-coord. K and 7- and 9-coord. Ba atoms. Phase in the $K_2O/BaO/SiO_2$ system. Cryst. SiOSi 180°, 163°.

Cervantes-Lee, F.J. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2099 (*synth, cryst struct*)

$Ba_9FFe_2H_{12}O_{32}Si_{12}Ti_2$ IC-001428

Traskite

[60650-96-6]

$(Ca,Sr)Ba_{24}(Mg,Mn,Fe,Al,Ti)_{16}[Si_2O_7]_6[Si_{12}O_{36}](O,OH)_{30}Cl_6.14H_2O$

M 2323.4

Highly idealised formula given. Unbranched, single ring silicate. (12 SiO_4 tetrahedra per ring). Also formulated as $Ba_9Fe_2Ti_2(SiO_3)_{12}(OH,Cl,F).6H_2O$. Mineral. Brown-red cryst.

Malinovskii, Yu.A. *et al*, *Sov. Phys.-Dokl.* (*Engl. Transl.*), 1976, **21**, 426 (*cryst struct*)

Pararennykh, A.S., *Mineral. Zh.*, 1979, **1**, 3 (*ir*)

$Ba_{10}Ca_2F_{10}MnO_{30}Si_{10}Ti$ IC-001429

Muirite

[12173-99-8]

$Ba_{10}(Ca,Mn,Ti)_4[Si_8O_{24}](Cl,F,O,OH)_{12}.4H_2O$

M 2507.0

Unbranched, single ring silicate with 8 SiO_4 units. Also formulated as $Ba_{10}Ca_2MnTiSi_{10}O_{30}(OH,Cl,F)_{10}$. Mineral, found in sanbornite-bearing metamorphic rocks in California. Orange cryst.

Khan, A.A. *et al*, *Science* (*NY*), 1971, **173**, 916 (*cryst struct*)

Malinovskii, Yu.A. *et al*, *Probl. Kristallologii*, 1976, 143 (*cryst struct*)

Pavarennykh, A.S., *Mineral. Zh.*, 1979, **1**, 3 (*ir*)

Be IC-001430

Beryllium

Glucinium. Glucinum

[7440-41-7]

Be

M 9.0

Atomic No 4. Ground state electron config. $[He]2s^2$. There are 6 isotopes of which only ^9Be is naturally occuring. Discovered in 1797 by L.N. Vauquelin and independently isolated in 1828 by F. Wöhler (Berlin) and A.H.B. Bussy (Paris). Abundance: 2 ppm (earth's crust), 5×10^{-5} ppm (sea water). The α-form (hcp) transforms into β-form (bcc) at 1250°. Main mineral is beryl (emerald). Metal obt. by electrolysis of BeF_2/MF mixt., or of pure $BeCl_2$ or from $BeCl_2$ + K, BeF_2 + Mg. Commercially available. Neutron multiplier in fusion reactors. Used as implant (dopant) in semiconducting devices (GaAs, InP, InAs). Forms alloys with Cu, Ni. Rel. soft silvery-white, lustrous metal; brittle at r.t., ductile at red heat. Unreactive to H_2O and air; dissolves vigorously in dil. acids. Reacts with halogens and higher chalcogens at high temp. Cold conc. HNO_3 passivates Be. Reacts with aq. alkalis → H_2. Mp 1287-1292°. Bp_5 2970° (*ca.* 2500°).

▷ Highly toxic: suspected carcinogen. The powdered metal is a fire and explosion hazard. DS1750000.

[14452-60-9, 57348-29-5, 58500-89-3]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1923, **4**, 204 (*rev, bibl*)

Gmelin Handbook Inorg. Chem., Syst. No. 26, 1930; *Suppl.*, 1986, **A1** (*rev, bibl*)

Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 565 (*history*)

Mackay, K.J.H. *et al*, *J. Nucl. Mater.*, 1963, **8**, 263 (*cryst struct*)

Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, 887 (*synth*)

Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 531 (*rev*)

Talbot, S., *Monogr. Met. Haute Purete*, 1977, **2**, 88 (*rev, synth, struct, props*)

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **3**, 803, 824 (*rev, bibl*)

Joenssen, S., *J. Crystal Growth*, 1983, **63**, 116 (*allotropy*)

Granger, P., *NMR Newly Accessible Nuclei*, (Ed. Laszlo, P.), Academic Press, N.Y., 1983, **2**, 385 (*Be-9 nmr*)

Preuss, O.P., *Fusion Technol.*, 1985, **8**, 1137 (*tox*)

Berwald, D.H. *et al*, *Fusion Technol.*, 1985, **8**, 1143 (*uses, fusion*)

Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 117 (*rev*)

Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 30.

Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 428 (*tox, haz*)

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 85 (*haz*)

$BeBr_2$ IC-001431

Beryllium bromide ($BeBr_2$), 8CI

Beryllium dibromide

[7787-46-4]

$BeBr_2$

M 168.8

Prepd. by reaction of metallic Be with Br_2 vapour (entrained in an Ar gas stream) at 50°. Deliquescent colourless orthorhombic cryst. V. sol. H_2O; sol. EtOH, Et_2O; insol. C_6H_6. Mp 508°. Subl. 490°. ΔH_f° −356 kJ mol^{-1}; ΔG_f° −337 kJ mol^{-1}; S° 100 J K^{-1} mol^{-1}.

▷ Highly toxic, suspected carcinogen.

Balaban, A.T. *et al*, *Rev. Chim. Acad. Repub. Pop. Roum.*, 1963, **8**, 139; *CA*, 1964, **60**, 12871a (*synth*)

Semenenko, K.N. *et al*, *Zh. Strukt. Khim.*, 1963, **4**, 67 (*cryst struct*)

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*uses*)

Snelson, A., *J. Phys. Chem.*, 1968, **72**, 250 (*matrix ir*)

Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 361 (*thermochem data*)

$BeCaFNaO_6Si_2$ IC-001432

Leucophanite

Leucophane

[12291-82-6]

$Na[BeCaF(SiO_3)_2]$

M 243.2

Unbranched, single chain silicate (4 SiO_4 units per chain). Mineral. White or light yellow cryst. Also formulated as $(Na,Ca)_2BeSi_2(O,F,OH)_7$.

[12198-56-0]

Cannillo, E. *et al*, *Acta Crystallogr.*, 1967, **23**, 255 (*cryst struct*)

Coda, A., *Rend. Soc. Ital. Mineral. Petrol.*, 1969, **25**, 195.

Shatskaya, V.T. *et al*, *Tr. Mineral. Muz., Akad. Nauk SSSR*, 1969, **19**, 239 (*synth, ir*)

$BeCa_2O_7Si_2$ IC-001433

Gugiaite

[13598-11-3]

$Ca_2Be[Si_2O_7]$

M 257.3

Mineral, found in skarn at Gugia, China. Colourless tetragonal cryst.

Burt, D.M., *Econ. Bull. Soc. Econ. Geol.*, 1975, **70**, 1279 (*synth*)

Kumata, M. *et al*, *Neues Jahrb. Mineral., Abh.*, 1982, **143**, 210 (*synth, cryst struct*)

$BeCa_4Ce_4FH_8Na_4O_{48}Si_{13}$ IC-001434

Semenovite, 9CI

[12777-32-1]

$(Ca,Na)_8Na_{0-2}Ln_2H_x(Fe,Mn,Zn,Ti)[(Si,Be)_{10}(O,F)_{24}]_2$

M 1981.8

Mineral. A layer silicate. Also formulated as $(Ca,Ce,La,Na)_{10-12}(Fe^{II},Mn)(Si,Be)_{20}(O,OH,F)_{48}$. Occurs in cavities on one epi-eudidymite bearing adbitite at Ilimaussaq, Greenland. Brown or grey orthorhombic cryst.

Petersen, O.V. *et al*, *Lithos*, 1972, **5**, 163 (*mineral*)

Mazzi, F. *et al*, *Am. Mineral.*, 1979, **64**, 202 (*cryst struct*)

$BeCl_2$ IC-001435

Beryllium chloride ($BeCl_2$), 8CI

[7787-47-5]

$BeCl_2$

M 79.9

Prepd. by direct reaction of Be + Cl_2 at 350-400°. Manuf. by treatment of Na_2BeF_4, obtained from a mixt. of beryl ore and Na_2SiF_6 heated to 600-820°,with a chlorinating agent (BCl_3, CCl_4, $COCl_2$, $SiCl_4$). Metallothermic reduction of $BeCl_2$ is used for beryllium manuf. Colourless orthorhombic cryst.; deliquescent. Undergoes transition to high temp. orthorhombic polymorph. at 403°. V. sol. H_2O, EtOH, Et_2O, Py; spar. sol. C_6H_6, $CHCl_3$, CS_2; insol. NH_3, Me_2CO. Mp 415°. Bp 520°. ΔH_f° −496 kJ mol^{-1}; ΔG_f° −450 kJ mol^{-1}; S° 75.8 J K^{-1} mol^{-1}.

▷ Highly toxic; suspected carcinogen. DS2625000.

Tetrahydrate: [13466-27-8].

$BeCl_2H_8O_4$ M 151.9

Cryst. (aq. soln.). Readily loses two H_2O molecules to form dihydrate at 60°. Layered struct. built up from $BeCl_2.2H_2O$ moieties with spaces filled with H_2O molecules.

▷ DS2675000.

Tetraammine complex:

$BeCl_2H_{12}N_4$ M 148.0

Colourless orthorhombic cryst.; dec. on heating with NH_3 loss forming $BeCl_2$.

Rundle, R.E. *et al*, *J. Chem. Phys.*, 1952, **20**, 132 (*cryst struct*)

Bobovich, Ya.S., *Opt. Spektrosk.*, 1961, **11**, 161; *CA*, 1962, **56**, 114f (*raman*)

Balaban, A.T. *et al*, *Rev. Chim. Acad. Repub. Pop. Roum.*, 1963, **8**, 139; *CA*, 1964, **60**, 12871a (*synth*)

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*uses*)

U.S. Pat., 3 146 065, (1964); *CA*, **61**, 11666a (*manuf*)

Semenenko, K.N., *CA*, 1965, **63**, 17428e (*tetraammine, cryst struct*)

Grigor'ev, A.I. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **160**, 383 (*tetraammine, ir, raman*)

Semenenko, K.N. *et al*, *Zh. Neorg. Khim.*, 1965, **10**, 77 (*tetrahydrate, cryst struct*)

Leone, W.L. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 3589 (*tetrahydrate, synth*)

Snelson, A., *J. Phys. Chem.*, 1968, **72**, 250 (*matrix ir*)

Sipachev, V.A. *et al*, *CA*, 1971, **73**, 55518 (*ir*)

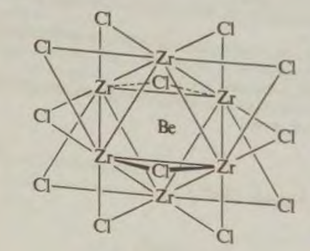
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 367 (*polymorph, thermochem data*)

$BeCl_{12}Zr_6$ IC-001436

(Beryllium)dodeca-μ-chlorohexazirconium

Beryllium zirconium chloride ($BeZr_6Cl_{12}$)

[96929-11-2]



one Cl not shown

M 981.7

Isol. as complex with KCl in which zirconium clusters are linked by chloride bridges. Primarily indexed as $Cl_{13}Zr_6^{3\ominus}$ in CAS.

KCl complex: [96929-12-3]. *Beryllium potassium dodeca-μ-chlorochlorohexazirconate(3−), 11Cl*

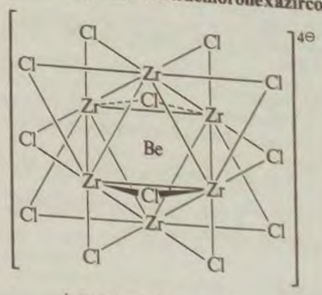
$BeCl_{13}KZr_6$ M 1056.3

Synth. by heating $ZrCl_4$ + Zr + Be + KCl in a sealed Ta tube at 700-860° for 2-3 weeks. Red-brown solid.

Ziebarth, R.P. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 4571 (*synth, cryst struct*)

$BeCl_{16}Zr_6^{4\ominus}$ IC-001437

(Beryllium)dodeca-μ-chlorotetrachlorohexazirconate(4−)



4 terminal Cl not shown

M 1123.5 (ion)

Indexed as a $Cl_{16}Zr_6^{4\ominus}$ cluster by CAS.

Tetra-Na salt: [96929-25-8]. *Beryllium tetrasodium dodeca-μ-chlorotetrachlorohexazirconate(6−), 11Cl*

$BeCl_{16}Na_4Zr_6$ M 1215.5

Synth. from Zr, $ZrCl_4$, NaCl and Be in a sealed Ta capsule at 700-860°. Black cryst. Struct. descr. as distorted M_6X_{12} version of $(Mo_6Cl_8)Cl_4$ struct.

Ziebarth, R.P. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 4571 (*synth, struct*)

BeCu IC-001438

Copper beryllium (1:1)

γ-Copper-beryllium

[12232-11-0]

BeCu

M 72.5

CsCl-type struct. Also designated β'.

Kossolopow, G.F. *et al*, *Metallwiss., Metalltech.*, 1935, **14**, 45 (*struct*)
Misch, L., *Z. Phys. Chem., Abt. B*, 1935, **29**, 42 (*struct*)
Domngang, S., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1973, **276**, 701 (*nmr*)
Ramachandran, K.N. *et al*, *J. Vac. Sci. Technol.*, 1973, **10**, 1068 (*x-ray spec*)
Moruzzi, V.L. *et al*, *Phys. Rev. B*, 1974, **10**, 4856 (*charge transfer*)
Iguchi, Y., *Program Ext. Abstr.- Int. Conf. Phys. X-ray Spectra*, 1976, 1976, 130 (*x-ray spec*)
Smithells Metals Reference Book, 6th Ed., Butterworths, London, 1983 (*struct, props*)

IC-001439

BeF_2

Beryllium fluoride (BeF_2)

[7787-49-7]

BeF_2

M 47.0

Hexagonal. Prepd. by thermal dec. of $(NH_4)_2BeF_4$ obt. by reaction of BeO with NH_4F or $NH_4.HF_2$. Component of FLiBe - a nuclear fusion reactor blanket tritium breeding material containing LiF and BeF_2. Component of halide glasses. Metallothermic reduction of BeF_2 is used for beryllium manuf. Colourless hexagonal cryst. Undergoes transition from low temp. quartz to high temp. quartz struct. types at 227°. Readily forms glasses. V. sol. H_2O; spar. sol. EtOH. Mp 552°. Subl. 800°. ΔH_f° −1025 kJ mol^{-1}; ΔG_f° −979 kJ mol^{-1}; S° 53.4 J K^{-1} mol^{-1}.

▷ Highly toxic, suspected carcinogen. DS2800000.

Novoseiova, A.V. *et al*, *CA*, 1957, **51**, 5615g (*cryst struct, polymorph*)
Brunton, G.D. *et al*, *U.S. At. Energy Comm., Rept. ORNL-3761*, 1965 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1966, **9**, 552 (*uses*)
Bell, R.J. *et al*, *Proc. Phys. Soc. London, Solid State Physics*, 1968, **1**, 299 (*ir, raman*)
Daenner, W., *Reaktortagung*, 1972, 747; *CA*, 1973, **76**, 10619 (*use*)
Johnson, A.B. *et al*, *BNWL-SA-5164, Report 1974*; *CA*, 1975, **83**, 67223 (*use*)
Baldwin, C.M. *et al*, *J. Non-Cryst. Solids*, 1981, **43**, 309 (*glass formn*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, Suppl. 1, 1985, **14**, 372 (*polymorph, thermochem data*)

$BeFe_3H_2O_{11}Si_3$

IC-001440

Beryllium iron hydroxide silicate ($BeFe_3(OH)_2(Si_3O_9)$)

[12449-14-8]

$Fe_3Be[Si_3O_9](F,OH)_2$

M 438.8

$F^\ominus$ and $OH^\ominus$ ions are interchangeable. Synthetic, unbranched, single chain silicate (wollastonite-like Si—O chain based on Fe). Obt. by hydrothermal treatment of Be by HF or AlF_3 with Fe leached from the autoclave walls. Transparent copper-yellow cryst.

Bakakin, V.V. *et al*, *Kristallografiya*, 1969, **14**, 1063; 1970, **15**, 1144; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1970, **14**, 920; 1971, **15**, 999 (*cryst struct*)

BeH_2O_2

IC-001441

Beryllium hydroxide ($Be(OH)_2$), 8CI

[13327-32-7]

$Be(OH)_2$

M 43.0

Orthorhombic, struct. resembles ε-$Zn(OH)_2$. Freshly precipitated $Be(OH)_2$ is an amorph. jelly-like material which is transformed with time into a much less sol. modification. Hydrol. of beryllium(*II*) in aq. salt solns. results in the formation of $Be_2(OH)^{3\oplus}$, $Be_3(OH)_3^{3\oplus}$ and $Be_5(OH)_7^{3\oplus}$ species. Prep. by hydrol. of $Be^{2\oplus}$ salts in aq. $[NH_4]Cl$ or NaCl soln. Colourless orthorhombic cryst. Dec. on heating with H_2O loss forming BeO (>1000°). Pract. insol. H_2O (3 × 10^{-5} g per 100 cm^3 at 25°). ΔH_f° −906 kJ mol^{-1}, ΔG_f° −818 kJ mol^{-1}; S° 50 J $K^{-1}mol^{-1}$.

▷ Highly toxic; suspected carcinogen. DS3150000.

Dihydrate: [65860-57-3].
BeH_6O_4 M 79.0
Colourless cryst., dec. on heating with H_2O loss.

Haber, F. *et al*, *Z. Anorg. Allg. Chem.*, 1940, **38**, 377 (*synth*)
Seitz, A. *et al*, *Z. Anorg. Allg. Chem.*, 1950, **261**, 94 (*cryst struct*)
Mesmer, R.E. *et al*, *Inorg. Chem.*, 1967, **6**, 1951 (*hydrol*)
Walrafen, G.E. *et al*, *Appl. Spectrosc.*, 1979, **33**, 524 (*dihydrate, ir, raman*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 389 (*thermochem data*)

BeI_2

IC-001442

Beryllium iodide (BeI_2), 8CI

Beryllium diiodide

[7787-53-3]

BeI_2

M 262.8

Prepd. by heating metallic Be or beryllium carbide in a stream of hydrogen and iodine at 750-1100°. Colourless orthorhombic cryst. Transforms to a second orthorhombic modification at ~350°. Mp 480°. Bp 590°. ΔH_f° −189 kJ mol^{-1}; ΔG_f° −187 kJ mol^{-1}; S° 121 J K^{-1} mol^{-1}.

▷ Highly toxic; suspected carcinogen.

Semenenko, K.N. *et al*, *Zh. Strukt. Khim.*, 1963, **4**, 67 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*uses*)
Snelson, A., *J. Phys. Chem.*, 1968, **72**, 250 (*matrix ir*)
Izhvanov, L.A. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1971, 109 (*synth*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 392 (*thermochem data*)

$BeK_2O_{10}Si_4$

IC-001443

Potassium beryllosilicate ($K_2BeSi_4O_{10}$)

Beryllium potassium silicate ($BeK_2(Si_4O_{10})$)

[76572-94-6]

$K_2[BeSi_4O_{10}]$

M 359.5

A single layer silicate. Struct. contains $[BeSi_4O_{10}]^{2\ominus}$ ions, formed from linkage of BeO_4 and SiO_4 tetrahedra, and $K^\oplus$ ions. Cryst.

Balko, V.P. *et al*, *Dokl. Akad. Nauk SSSR*, 1980, **255**, 565; *CA*, **94**, 94050g (*cryst struct*)

BeN_2O_6

IC-001444

Beryllium nitrate ($Be(NO_3)_2$)

Nitric acid, beryllium salt, 8CI

[13597-99-4]

$Be(NO_3)_2$

M 133.0

Prepd. by thermal dec. of $Be(NO_3)_2.2N_2O_4$ The dissolution of beryllium metal in a mixt. of MeOH and CCl_4 followed by evaporation of the solv. yields beryllium powder which reacts readily with aq. HNO_3 to form $Be(NO_3)_2$ solns. Deliquescent white amorphous solid. ΔH_f° −678 kJ mol^{-1}.

▷ Highly toxic, suspected carcinogen. DS3675000.

Trihydrate: [7787-55-5].
$BeH_6N_2O_9$ M 187.0
Deliquescent pale yellow cryst. V. sol. H_2O, EtOH. Mp 60°. Bp 142°. ΔH_f° −788 kJ mol^{-1}.

Tetrahydrate: [13510-48-0].
$BeH_8N_2O_{10}$ M 205.0
Tetragonal cryst.

Bis(dinitrogen tetroxide) complex: Obt. by treating $BeCl_2$ with a mixt. of N_2O_4 and EtOAc. Dec. on heating → Hexakis[μ-(nitrato-*O*:*O'*)]-μ_4-oxotetraberyllium, IC-001462.

Addison, C.C. *et al*, *J. Chem. Soc.*, 1963, 1220 (*synth, ir*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*uses*)
Addison, C.C. *et al*, *J. Chem. Soc. A*, 1966, 1524 (*uv-vis*)
U.S. Pat., 3 574 533, (1971); *CA*, **74**, 128274 (*manuf*)
Ribar, B. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1972, **136**, 159 (*tetrahydrate, cryst struct*)

$BeNa_2O_6Si_2$

IC-001445

Chkalovite

[13598-20-4]

$Na_6Be_3[Si_6O_{18}]$

M 207.1

Unbranched, single chain silicate (6 SiO_4 tetrahedra per chain). Mineral. Cryst.

Bukin, G.V., *Geol. Geofiz.*, 1968, 124 (*synth*)
Moleva, V.A., *Khim. Anal. Formuly Miner.*, 1969, 110 (*cryst struct*)
Simonov, M.A. *et al*, *Sov. Phys.-Dokl. (Engl. Transl.)*, 1975/6, **20**, 805 (*cryst struct*)
Kiseleva, I.A. *et al*, *Vestn. Mosk. Univ., Ser. 2: Khim.*, 1984, **25**, 278 (*thermodyn props*)

BeO

IC-001446

Beryllium oxide (BeO)

[1304-56-9]

BeO

M 25.0

Deformed wurtzite struct. type. Prepd. by calcination of $Be(OH)_2$ or $BeSO_4$ or by oxidation of beryllium metal powders. Commercially available. Used in production of ceramics, particularly in combination with silicon carbide, silicon nitride. Used in thermoluminescent dosimeters. Extensively used as a refractory material. White hexagonal cryst. Piezoelectric and pyroelectric. Undergoes hexagonal to tetragonal transition at 2100°. Dissolves in conc. H_2SO_4 and in fused KOH. Spar. sol. H_2O (2 × 10^{-5} g per 100 cm^3 at 30°). Mp 2507°. Bp *ca.* 3900°. ΔH_f° −608 kJ mol^{-1}; ΔG_f° −579 kJ mol^{-1}; S° 13.8 J K^{-1} mol^{-1}.

▷ Highly toxic, suspected carcinogen. DS4025000.

Mineral-form [13598-21-5]
Bromellite
Mineral found in calcite veinlets at sites in Sweden and USSR. Transparent, white trigonal cryst.

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*uses*)
Smith, D.K. *et al*, *J. Electrochem. Soc.*, 1964, **111**, 78 (*cryst struct*)
Smith, D.K. *et al*, *Acta Crystallogr.*, 1965, **18**, 4035 (*polymorphs*)
Tochilin, E. *et al*, *Health Phys.*, 1969, **16**, 1 (*use, dosimeter*)
Walrafen, G.E. *et al*, *Appl. Spectrosc.*, 1979, **33**, 524 (*ir, raman*)
Kaczynski, D.J. *et al*, *Ceram. Eng. Sci. Proc.*, 1985, **6**, 1261 (*rev, bibl, ceramics*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 397 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 407C (*haz, tox*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 433 (*tox*)

BeO_4S

IC-001447

Beryllium sulfate ($BeSO_4$)

Sulfuric acid, beryllium salt, 8CI

[13510-49-1]

$BeSO_4$

M 105.0

Struct. resembles BPO_4. Prepd. by thermal dehyd. of the tetrahydrate *in vacuo*. Cyclocondensation catalyst for conversion of anilines to indoles. Colourless tetragonal cryst., hygroscopic. Undergoes polymorphic transitions at 590° and 635°. On further heating dissoc. without melting to BeO, SO_3, SO_2 and O_2. Insol. H_2O. ΔH_f° −1201 kJ mol^{-1}; ΔG_f° −1089 kJ mol^{-1}; S° 78 J K^{-1} mol^{-1}.

▷ Highly toxic, suspected carcinogen. DS4800000.

Monohydrate: [14214-99-4].
Dihydrate: [14215-00-0].
Tetrahydrate: [7787-56-6]. *Tetraaquaberyllium(2+) sulfate*
BeH_8O_8S M 177.1
Synth. by cryst. from an aq. soln. of $BeSO_4$ obt. by careful neutralisation of BeO or $Be(OH)_2$ with aq. H_2SO_4. Commercially available. Colourless tetragonal cryst. dec. on heating with H_2O loss (−$2H_2O$ at 200°, −$4H_2O$ at 400°). V. sol. H_2O (42.5 g per 100 cm^3 at 25°; 100 g per 100 cm^3 at 100°). Comprises $[Be(H_2O)_4]^{2\oplus}$ cations + $SO_4^{2\ominus}$ anions. Piezoelectric. ΔH_f° −2424 kJ mol^{-1}; ΔG_f° −2081 kJ mol^{-1}; S° 234 J K^{-1} mol^{-1}.

▷ Highly toxic; suspected carcinogen. DS5000000.

Kokkoros, P.A., *Mineral. Petrogr. Mitt.*, 1958, **6**, 116 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*uses*)
Dance, I.G. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 304 (*cryst struct, tetrahydrate*)
Sikka, S.K. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 310 (*cryst struct, nd, tetrahydrate*)
Matsuda, S. *et al*, *Yogyo Kyokaishi*, 1971, **79**, 351 (*synth, tetrahydrate*)
Johnson, D.W. *et al*, *J. Phys. Chem.*, 1972, **76**, 1474 (*thermal dec, anhyd, tetrahydrate*)
Vasil'ev, V.G. *et al*, *Zh. Neorg. Khim.*, 1972, **17**, 625, 631 (*thermal dec, anhyd, tetrahydrate*)
Murthy, S.V., *Indian J. Phys., A*, 1977, **51**, 258 (*pmr, tetrahydrate*)
Japan. Pat., 81 150 062, (1981); *CA*, 1982, **96**, 68819 (*uses*)
Pigenet, C., *J. Raman Spectrosc.*, 1982, **13**, 66, 262 (*ir, raman, tetrahydrate*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 402 (*polymorph, thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 407D (*haz, tetrahydrate*)

BeS

IC-001448

Beryllium sulfide (BeS), 8CI

[13598-22-6]

BeS

M 41.0

Zinc blende-type struct. Prepd. by reaction of Be metal with H_2S in an autoclave. Semiconductor with band gap > 5.5eV. Moisture sensitive colourless cubic cryst. Hydrol. in H_2O with formation of $Be(OH)_2$ and H_2S. ΔH_f° −234 kJ mol^{-1}; ΔG_f° −233 kJ mol^{-1}; S° 37 J K^{-1} mol^{-1}.

▷ Highly toxic, suspected carcinogen.

Stanitzky, E., *Anal. Chem.*, 1956, **28**, 915 (*cryst struct*)
Yim, W.M. *et al*, *J. Phys. Chem. Solids*, 1972, **33**, 501 (*synth*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 406 (*thermochem data*)

IC-001449

$Be_2Ca_2Fe_3H_2Mg_2O_{24}PbSi_6$

Joesmithite, 9CI

[12417-03-7]

$Be_2Ca_2(Ca,Pb)(Fe,Mg)_2[SiO_4]_2[Si_2O_6]_2O_2(OH)_2$

M 1076.0
Mineral. Struct. resembles an amphibole but is a hybrid consisting of $[Si_2O_6]_\infty$ pyroxene chains and $[SiO_4]$ tetrahedra. Also formulated as (Ca,Pb) $Ca_2(Mg,Fe^{II},Fe^{III})_5Si_6Be_2O_{22}(OH)_2$. Found at Långban, Sweden in hematite-magnetite-chefferite skarn assemblage. Black prisms with pale brown streak.

Moore, P.B., *Mineral. Mag.*, 1968, **36**, 876 (*cryst struct*)
Moore, P.B., *Am. Mineral.*, 1969, **54**, 577 (*mineral*)

IC-001450

$Be_2Ca_3H_2O_{12}Si_3$

Aminoffite

Beryllium calcium hydroxide silicate ($Be_2Ca_3(OH)_2(Si_3O_{10})$)

[12251-61-5]

$Be_2Ca_3[Si_3O_{10}](OH)_2$

M 416.5
Unbranched oligosilicate (3 SiO_4 tetrahedra per unit). Mineral, found at sites in Sweden and USSR. Colourless to pale yellow transparent cryst.

Coda, A. *et al*, *Atti R. Accad. Naz. Lincei, Rend. Cl. Sci. Fis., Mat. Nat.*, 1967, **43**, 225 (*cryst struct*)
Coda, A., *Rend. Soc. Ital. Mineral. Petrol.*, 1969, **25**, 195.

IC-001451

$Be_2FeGdO_{10}Si_2Y$

Gadolinite

[12196-15-5]

$(Y,M)_2Fe^{II}Be_2O_2(SiO_4)_2$ M = rare earth,esp. Gd

M 536.1
Idealised formula given. Original Gd ore, also contains other rare earths. Found in N. Europe, USSR, USA, Alps. Dark green to black cryst. usually brittle, hard.

[66143-35-9]

Compr. Inorg. Chem., Pergamon, Oxford, 1973, **4**, 46.
Gorobets, B.S. *et al*, *Izv. Akad. Nauk SSSR, Ser. Geol.*, 1981, 117; *CA*, **95**, 51924 (*luminescence*)
Miyawaki, R. *et al*, *Am. Mineral.*, 1984, **69**, 948 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **A8**, 72 (*rev*)
Bernardino, T., *Rev. Mineral Ital.*, 1985, 84 (*uv-vis*)

IC-001452

Be_2GeO_4

Beryllium germanate (Be_2GeO_4)

Beryllium germanium oxide (Be_2GeO_4)

[12232-39-2]

Be_2GeO_4

M 154.6
Phenakite struct. Solid.

Schutz, W., *Z. Phys. Chem., Abt. B*, 1936, **31**, 292 (*struct*)

IC-001453

$Be_2H_2Na_2O_{16}Si_6$

Eudidymite, 9CI

[16224-19-4]

$Na_2Be_2[Si_6O_{15}].H_2O$

M 490.5
Mineral. Dimorphous with epididymite. A double chain silicate. Also formulated as $NaBeSi_3O_7(OH)$. Occurs in nepheline-syenite pegmatites in Norway, Greenland and USSR in assoc. with dimorph. Usually white or colourless monoclinic cryst.

Dimorph.-form [15038-95-6]
Epididymite
Double-chain silicate. Brittle orthorhombic cryst., usually white.

[37349-75-0, 60867-27-8]

Robinson, P.D. *et al*, *Am. Mineral.*, 1970, **55**, 1541 (*cryst struct, epididymite*)
Fang, J.H. *et al*, *Am. Mineral.*, 1972, **57**, 1345 (*cryst struct, eudidymite*)

IC-001454

$Be_2H_4Na_4O_{20}Si_6Sn$

Sorensenite

[11118-38-0]

$Na_4Be_2Sn[Si_3O_9]_2.2H_2O$

M 721.2
Unbranched, single chain silicate (3 SiO_4 units per chain). Mineral. Colourless cryst.

Metcalf-Johansen, J. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 2553 (*cryst struct*)
Maksimova, N.V. *et al*, *Konst. Svoistva Miner.*, 1976, **10**, 9 (*cryst struct*)
Graft, M.L. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1982, **266**, 217.

IC-001455

$Be_2K_2O_{15}Si_6$

Beryllium potassium silicate ($Be_2K_2(Si_6O_{15})$)

Potassium beryllosilicate

$K_2Be_2[Si_6O_{15}]$

M 504.7
K analogue of eudidymite. A single-layer silicate.

Naumova, I.S. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1976, **229**, 856; *CA*, **85**, 170018 (*cryst struct*)

IC-001456

$Be_2Na_2O_9Si_3$

Beryllium sodium silicate ($Be_2Na_2(Si_3O_9)$)

[80777-49-7]

$Na_2Be_2[Si_3O_9]$

M 292.2
Synthetic, unbranched, monocyclosilicate. (3 SiO_4 tetrahedra per ring). Known since ~1890. Orthorhombic. Transparent colourless cryst.

Grinderow, D. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 62 (*cryst struct*)

Be_2O_4Si

Beryllium silicate (Be_2SiO_4) **IC-001457**

Beryllium orthosilicate

[15191-85-2]

$Be_2[SiO_4]$

M 110.1
Synth. by heating SiO_2 + BeO to 1500° in the presence of a mineralising agent. Cryst. Dec. >1560°→ BeO + SiO_2.

▷ VV8925000.

Mineral-form [13598-00-0]
Phenakite. Phenacite
Be_2O_4Si M 110.1
Structural prototype with 4-coord. Be. Occurs in granite pegmatites, greisens, hydrothermal and Alpine veins, in many localities. Colourless, yellow, pink, pinkish red, brown, trigonal cryst.

Bragg, W.L. *et al*, *Z. Kristallogr.*, 1930, **72**, 518 (*cryst struct*)
Zachariasen, W.H., *Kristallografiya*, 1971, **16**, 1161; *CA*, **70**, 51334p (*cryst struct*)
Piir, K.Yu. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 2061 (*synth*)
Handke, M. *et al*, *J. Mol. Struct.*, 1982, **79**, 353 (*ir, raman*)
Kiseleva, I.A. *et al*, *Geokhimiya*, 1983, 310; *CA*, **98**, 146721f (*thermodyn*)
Magi, M. *et al*, *J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)

$Be_2O_7Rb_2Si_2$

Beryllium rubidium silicate ($Be_2Rb_2(Si_2O_7)$) **IC-001458**

Rubidium beryllosilicate ($Rb_2(Be_2Si_2O_7)$)

[59514-41-9]

$Rb_2Be_2[Si_2O_7]$

M 357.1
Struct. comprises Si_2O_7 groups linked at their corners by Be atoms to form an infinite frame anion of empirical formula $(Be_2Si_2O_7)^{2\ominus}$ with planar BeO_3 groups. $Rb^\oplus$ in either 13 or 14 coordination. Angle: SiOSi 171°. Synth. from Rb_2CO_3, BeO and quartz. Cryst. Above 1000-1100° loses rubidium oxide.

Havie, R.A. *et al*, *Nature (London)*, 1976, **259**, 473 (*synth, cryst struct*)
Havie, R.A. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 381 (*cryst struct*)

Be_3N_2

Beryllium nitride (Be_3N_2), 8CI **IC-001459**

[1304-54-7]

Be_3N_2

M 55.0
Cubic; isotypic with anti-Mn_2O_3 (Mg_3P_2). Prepd. by direct reaction of the elements at elevated temps. (900-1100°). Used in the preparation of ternary beryllium silicon nitrides, e.g. $BeSiN_2$. Moisture sensitive pale grey cubic cryst. Hydrol. in H_2O with formation of $Be(OH)_2$ and evolution of NH_3. Undergoes a cubic-hexagonal transformation in the presence of silicon nitride at >1400°. Mp 2200°. ΔH_f° −588.3 kJ mol^{-1}; ΔG_f° −532.9 kJ mol^{-1}; S° 34.1 J K^{-1} mol^{-1}.

▷ Highly toxic; suspected carcinogen.

Stackelberg, M. *et al*, *Z. Phys. Chem., Abt. B*, 1933, **22**, 305 (*cryst struct*)
Eckerlin, P. *et al*, *Z. Anorg. Allg. Chem.*, 1960, **304**, 218 (*polymorphs*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*uses*)
Juza, R. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1966, **70**, 1103 (*synth*)
Eckerlin, P. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **353**, 113 (*uses*)
Hall, D. *et al*, *Z. Anorg. Allg. Chem.*, 1969, **369**, 108 (*polymorphs*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 414 (*thermochem data*)

$Be_4Ca_6F_4Na_2O_{24}Si_8$

Meliphanite, 9CI **IC-001460**

Melinophane

[12440-99-2]

$(Na,Ca)_4Ca_4Be_4[Si_2O_{20}][SiO_4]F_4$

M 1007.1
Mineral. A branched layer silicate. Also formulated as $(Ca,Na)_2Be(Si,Al)_2(O,OH,F)_7$. Occurs in nepheline-syenite pegmatites. Also found in cavities in skarn rocks and disseminated in melanite. Yellow or colourless tetragonal cryst.

Dal Negro, A. *et al*, *Acta Crystallogr.*, 1967, **23**, 260 (*cryst struct*)

$Be_4H_2O_9Si_2$

Bertrandite, 9CI **IC-001461**

[12161-82-9]

$Be_4Si_2O_7(OH)_2$

M 238.2
Mineral. A framework silicate. Occurs in granite pegmatites, greisens, and aplites. A phase in the $BeO/Al_2O_3/SiO_2/H_2O$ system. The principal ore of beryllium. Colourless, pale yellow, orthorhombic cryst.

▷ DS1225000.

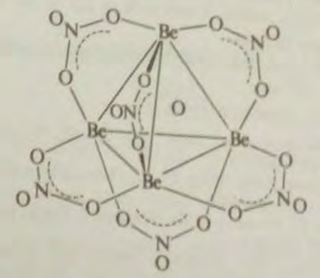
Levinson, A.A., *Am. Mineral.*, 1962, **47**, 67 (*occur*)
Barton, M.D., *Am. Mineral.*, 1986, **71**, 277 (*phase equilibria*)
Downs, J.W. *et al*, *Am. Mineral.*, 1987, **72**, 979 (*cryst struct*)

$Be_4N_6O_{19}$

Hexakis[μ-(nitrato-*O*:*O'*)]-μ_4-oxotetraberyllium, 11CI **IC-001462**

Basic beryllium nitrate. Tetraberyllium hexanitrate oxide. Beryllium nitrate oxide, 8CI. Beryllium oxynitrate

[12010-07-0]



M 424.0
Tetrahedron of Be with NO_3 bridging each edge, and central O atom. Prepd. by thermal dec. of $Be(NO_3)_2.2N_2O_4$ (via $Be(NO_3)_2$). Deliquescent white cubic cryst. Insol. non-polar solvs. Subl. 125°.

▷ Highly toxic, suspected carcinogen.

Addison, C.C. *et al*, *Proc. Chem. Soc., London*, 1961, 242 (*cryst struct*)
Addison, C.C. *et al*, *J. Chem. Soc.*, 1963, 1220 (*synth, ir*)
Sipachev, V.A. *et al*, *Polyhedron*, 1982, **1**, 820 (*electron impact studies*)
Tuseev, N.I. *et al*, *J. Mol. Struct.*, 1984, **125**, 277 (*ed, struct*)

$Be_{13}U$ IC-001463

Beryllium, compd. with uranium (13:1)

[12010-30-9]

UBe_{13}

M 355.1

Heavy-fermion compd. V. high conduction electron spec. heat. Alloy. Superconductor <0.86K (0.97K).

Lewis, J.R., *J. Met.*, 1961, **13**, 357 (*synth*)
Farkas, M. *et al*, *J. Nucl. Mater.*, 1968, **27**, 94 (*synth*)
Landgren, G. *et al*, *Phys. Rev. B*, 1984, **29**, 493 (*condy*)
Goldman, A.I. *et al*, *Phys. Rev. B*, 1985, **32**, 6042 (*struct*)
Ott, H.R., *Handbook on the Physics and Chemistry of the Actinides*, Freeman, A.J., *et al*, Eds., 1987, **5**, 85 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 55, Suppl. Vol., 1989, **B2**, 18 (*rev, bibl*)
Law, S., *New Sci.*, 1990, 57 (*rev*)

Bi IC-001464

Bismuth

[7440-69-9]

Bi

M 208.9

Atomic No. 83. Ground state electron config. [Xe] $4f^{14}5d^{10}6s^26p^3$. The only stable isotope is ^{209}Bi. Early history confused with that of Pb, Sn, Sb, Ag, but known in Middle Ages. Abundance: 0.008 ppm (earth's crust). Polymorphic. Occurs mainly as Bismuth oxide (Bi_2O_3), IC-001548 and Bismuth sulfide (Bi_2S_3), IC-001561. Heating oxide (Bi_2O_3) with KCN → metal. Isol. as by-product from Pb, Zn, Sn and Cu smelting processes. Used mainly in low melting metal alloys and in the manuf. of pharmaceutical compds. Reacts directly with halogens, O, or S. Attacked only slowly by HCl. Hot H_2SO_4 → sulfate, HNO_3 → nitrate + N oxides.

▷ EB2600000.

α-form

Rhombohedral lattice with Bi—Bi 307.2 (three nearer coplanar neighbours) and 352.9 pm, and BiBiBi 95.5°. Brittle, white cryst. metal with pinkish tinge, becoming plastic at 225°. Mp 271.4°. Bp 1564°.

High-pressure I-form

Monoclinic lattice. From α-Bi at 2.5×10^4 atm.

High-pressure II-form

Lattice form unknown. From the monoclinic form at 2.7×10^4 atm.

[12187-12-1, 12595-63-0, 12595-65-2]

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1927; *Suppl. Vol.*, 1964 (*rev, bibl*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 586 (*rev, bibl*)
Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 91 (*history*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 547 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 596 (*props*)
Edel'man, V.S., *Adv. Phys.*, 1976, **25**, 555 (*props*)
Bastow, T.J. *et al*, *Solid State Commun.*, 1976, **18**, 955 (*nqr*)
Lamparter, P. *et al*, *Z. Naturforsch., A*, 1976, **31**, 90 (*nd, struct, bibl*)
Carapella, S.C., *Encycl. Chem. Process. Des.*, 1977, **4**, 394 (*rev, manuf, phys props*)
McGilp, J.F. *et al*, *J. Phys. C*, 1977, **10**, 3445 (*pe*)
Fedotov, V.K. *et al*, *Fiz. Tverd. Tela (Leningrad)*, 1978, **20**, 1088; *Soviet Phys.: Solid State (Engl. Transl.)*, 1978, **20**, 628 (*nd*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **3**, 912; **19**, 639, 682 (*rev, bibl*)
George, S. *et al*, *J. Opt. Soc. Am.*, 1982, **72**, 589 (*ir*)
Granger, P., *NMR Newly Accessible Nuclei*, (Ed. Laszlo, P.), Academic Press, N.Y., 1983, **2**, 385 (*Bi-209 nmr*)
Takahashi, T. *et al*, *J. Non-Cryst. Solids*, 1984, **65**, 261 (*pe*)
Eberle, B. *et al*, *Surf. Sci.*, 1985, **156**, 751 (*raman*)
Reents, W.D. *et al*, *Chem. Phys. Lett.*, 1986, **125**, 324 (*ms*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 637 (*rev*)
Nomura, M. *et al*, *J. Phys. Soc. Jpn.*, 1986, **55**, 222 (*props*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 32.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 522 (*tox*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 87 (*haz*)

BiBrO IC-001465

Bismuth bromide oxide (BiBrO), 8CI

Bromooxobismuthine, *9CI. Bromooxobismuth*(III). *Bismuthyl bromide. Basic bismuth bromide*

[7787-57-7]

BiBrO

M 304.8

Tetragonal with layer-lattice struct. like BiClO. Bi—O 232.5, Bi—Br 316.9 pm. Obt. by diln. of conc. aq. soln. of $BiBr_3$. Used in manuf. of dry-cell cathodes. Sl. yellowish platelets or white powder. V. stable, melts only at red heat. Sol. conc. HBr aq.; insol. H_2O, EtOH. Sublimes.

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 705 (*rev, bibl*)
Rulmont, A., *Spectrochim. Acta, Part A*, 1972, **28**, 1287 (*ir*)
Davies, J.E.D., *J. Inorg. Nucl. Chem.*, 1973, **35**, 1531 (*ir, raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 599 (*synth*)
Bastow, T.J. *et al*, *J. Magn. Reson.*, 1977, **26**, 461 (*nqr*)
Ketterer, J. *et al*, *Acta Crystallogr., Sect. C*, 1986, **42**, 1098 (*cryst struct*)

BiBrS IC-001466

Bismuth bromide sulfide (BiBrS), 8CI

Bromothioxobismuthine, *9CI. Bromothioxobismuth*(III)

[14794-86-6]

BrBi=S

M 320.9

Orthorhombic. Each Bi atom is 7 coordinated by S (×3; 260.7-272.1 pm) and Br (×4; 303.3-353.9 pm). The Br and two S atoms are at vertices of a triangular prism. The third S is at apex of pyramid whose base is S_2Br_3 face of the triangular prism. The composite polyhedron is linked to another by a common S—S edge forming double chains of $(Bi_2S_4Br_2)_n$. Synth. from Bi + S + $BiBr_3$ at 530°; or from $BiBr_3$ + Bi_2S_3 at 460°. Red-brown (dark red) prisms or needles with metallic sheen. Mp 450°. Ferroelectric: photoconductor. At 300° loses $BiBr_3$, eventually forming Bi_2S_3 at 500°.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 753 (*rev, bibl*)
Kozáková, M. *et al*, *Z. Chem.*, 1966, **6**, 431 (*synth*)
Pikka, T. *et al*, *Fiz. Tverd. Tela (Leningrad)*, 1968, **10**, 3378; *Soviet Physics: Solid State*, 1968, **10**, 2668 (*electrical, optical props*)
Chepur, D.V. *et al*, *Phys. Status Solidi*, 1968, **30**, 461 (*ir*)
Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1969, **14**, 312 (*synth*)
Inorg. Synth., 1973, **14**, 160 (*synth*)
Kulieva, S.A. *et al*, *Azerb. Khim. Zh.*, 1974, 131; *CA*, **82**, 103882 (*synth, reactions*)
Furman, E. *et al*, *Phys. Rev. B: Solid State*, 1976, **13**, 1703 (*raman*)
Voutsas, G.P. *et al*, *Z. Kristallogr.*, 1984, **166**, 153 (*cryst struct*)

BiBrSe IC-001467

Bismuth bromide selenide (BiBrSe), 8CI

Bromoselenoxobismuthine, *9CI. Bromoselenoxobismuth*(III)

[22630-32-6]

BrBi=Se

M 367.8

Synth. from Bi + Se + Br_2 in gas phase, or from $BiBr_3$ + Bi_2Se_3, or similar reactants in HBr or Br_2 solv. at 260-370°/40-350 atm. Black needles or prisms. Mp 510° (475°). Possesses v. poor photoelectric props.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 772 (*rev, bibl*)
Horák, J. *et al*, *Krist. Tech.*, 1968, **3**, 241 (*synth, props*)
Chepur, D.V. *et al*, *Phys. Status Solidi*, 1968, **30**, 461 (*ir*)
Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1969, **14**, 312 (*synth*)
Popolitov, V.I. *et al*, *Phys. Status Solidi A*, 1970, **3**, K1 (*synth*)
Popolitov, V.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1983, **19**, 1651; *Inorg. Materials (Engl. Transl.)*, 1983, **19**, 1459 (*synth*)

BiBrTe IC-001468

Bismuth bromide telluride (BiBrTe), 8CI

Bromotelluroxobismuthine, *9CI. Bromotelluroxobismuth*(III)

[30382-76-4]

BrBi=Te

M 416.4

A layer struct. in which each Bi is surrounded by Br (2×) and Te (1×) from an upper layer, and Br (1×) and Te (2×) from lower layer, forming distorted octahedral coordination. Synth. from Bi + Te + Br_2, or from $BiBr_3$ + Bi + Te, at 400-500° under high press. (in HBr) or *in vacuo*. Hexagonal lamellae with mirror-like lustre. Mp 547° (congr.). Weak semi-conductor. Curie point ~160°.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 817 (*rev, bibl*)
Turjanica, I.D. *et al*, *Collect. Czech. Chem. Commun.*, 1968, **33**, 300 (*synth, uv*)
Chapur, D.V. *et al*, *Phys. Status Solidi*, 1968, **30**, 461 (*ir*)
Popolitov, V.I. *et al*, *Phys. Status Solidi A*, 1970, **3**, K1 (*synth*)
Onopko, L.V. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, **10**, 1137; *Inorg. Materials (Engl. Transl.)*, 1974, **10**, 975 (*synth*)
Matyáš, M. *et al*, *Phys. Status Solidi A*, 1980, **61**, 419 (*synth, props, ir*)

$BiBr_3$ IC-001469

Bismuth(*III*) bromide ($BiBr_3$)

Tribromobismuthine, *9CI. Tribromobismuth*(III). *Bismuth tribromide*

[7787-58-8]

$BiBr_3$

M 448.6

Polymorphic. Appears to be the only Group *V* trihalide which possesses molecular and polymeric structs. In vap., Bi—Br 263 pm, BrBiBr 100°. Synth. from BBr_3 + $BiCl_3$ or Bi_2O_3; Bi + Br_2; Br_2 + Bi_2S_3; Bi_2O_3 + CBr_4. Orange or golden-yellow deliquescent cryst. Melts to yellow to red liq. Vap. deep red. Mp 218°. Bp 441°, Bp 462°. Hydrol. (H_2O) to Bismuth bromide oxide (BiBrO), IC-001465, ΔH_f° −276 kJ mol^{-1}. Forms many complex halides with metal halides and hydrogen halides.

Mesitylene complex *(1:1)*: [18796-86-6]. *Tribromo(1,3,5-trimethylbenzene)bismuth*(III)
$C_9H_{12}BiBr_3$ M 568.8

Yellow solid. Mp 118°.

Hexamethylbenzene complex *(2:1)*: [110296-10-1]. *(Hexamethylbenzene)bis[tribromobismuth*(III)*]*
$C_{12}H_{18}Bi_2Br_6$ M 1059.6

Tetragonal yellow cryst. solid. Mp 162° dec.

α-form

Molecular. Monoclinic with trigonal-pyramidal geometry; Bi—Br 266 (3×), 332 (3×) pm. Also described as hcp Br atoms with Bi atoms in octahedral spaces. Transforms into β-form at 158°.

β-form

Monoclinic. Polymeric struct. with Bi—Br 282 pm.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 698 (*rev, bibl*)
Druce, P.M. *et al*, *J. Chem. Soc. A*, 1971, 3595 (*synth*)
Marconi, V.A. *et al*, *Appl. Spectrosc.*, 1973, **27**, 428 (*raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 599 (*synth*)
von Benda, H., *Z. Kristallogr.*, 1980, **151**, 271 (*cryst struct*)
Imperatori, P. *et al*, *J. Chem. Thermodyn.*, 1982, **14**, 461 (*ms*)
Novak, I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 635 (*pe*)
Schmidbaur, H. *et al*, *Chem. Ber.*, 1987, **120**, 1829, 1837 (*complexes*)

$BiBr_4H$ IC-001470

Hydrogen tetrabromobismuthate(*III*)(1−), 9CI, 8CI

$H[BiBr_4]$

M 529.6

Salts formed from $BiBr_3$ in HBr (aq.) + amine.

2-Methylpyridine salt: [18639-72-0].

Yellow cryst. Mp 207-208° (198°). Anion has polymeric chain struct. Distorted octahedral coordination of Br around Bi, with bridges of two Br atoms between Bi atoms. Free Bi—Br bonds are 263-265 pm. Bridging Bi—Br bonds, and angles, are irregular.

3-Methylpyridine salt: [28961-39-9].

Yellow cryst. Mp 220-222°.

Robertson, B.E. *et al*, *J. Phys. Chem.*, 1967, **71**, 3531 (*cryst struct*)
Whealy, R.D. *et al*, *Inorg. Chim. Acta*, 1970, **4**, 420 (*synth*)
Ahlijah, G.Y. *et al*, *J. Chem. Soc. A*, 1970, 326 (*synth, ir, raman*)
Hooper, H.A. *et al*, *Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)
Laane, J. *et al*, *Inorg. Chem.*, 1980, **19**, 44 (*ir, raman*)

$BiBr_5H_2$ IC-001471

Dihydrogen pentabromobismuthate(*III*)(2−), 9CI, 8CI

$H_2[BiBr_5]$

M 610.5

Salts obt. from $BiBr_3$ in HBr aq. + amine. Salts are insol. non-polar solvs.

Tetrahydrate: Synth. from $BiBr_3$ + HBr aq. at −10°. White needles.

Bis-isopropylamine salt: Yellow solid. Mp 285-288°.

Bis-butylamine salt: Yellow solid. Mp 249-251°.

Bis(4-methylpyridine) salt: [71733-94-3].

Yellow solid. Mp 186-189°.

Bis-piperidine salt: [18639-71-9].

Yellow solid. Anion consists of chains of octahedral $BiBr_6$ groups sharing vertices Bi—Br 267.1, 285.7 pm (terminal) 301.9, 312.5 (bridge). Dec. at 275° with melting to 304°.

Bis-morpholine salt: [69853-28-7].

Yellow salt. Stable in air.

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1927, 154; 1964, 704 (*rev, bibl*)
McPherson, W.G. *et al*, *J. Phys. Chem.*, 1968, **72**, 532 (*cryst struct*)

Whealy, R.D. *et al, Inorg. Chim. Acta*, 1970, **4**, 420 (*synth*)
Hooper, H.A. *et al, Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)
Cariati, F. *et al, Spectrochim. Acta, Part A*, 1978, **34**, 801 (*synth, ir, raman*)
Laane, J. *et al, Inorg. Chem.*, 1980, **19**, 44 (*ir, raman*)

IC-001472

$BiBr_5H_9N_2$

Diammonium pentabromobismuthate(2−), 9Cl, 8Cl
Pentabromobismuthate(III) *diammonium salt*

$(NH_4)_2BiBr_5$

M 644.5
May be dimeric.
Dihydrate: [21028-89-7].
$BiBr_5H_{13}N_2O_2$ M 680.6
Synth. from μ-[Carbonato(2−)-*O:O'*][dioxodibismuth], IC-002285 + $(NH_4)_2CO_3$ + HBr aq. Rhombic cryst.

Bartczak, T. *et al, Zesz. Nauk Politech. Lodz. Chem.*, 1966, No. 17, 21; *CA*, **69**, 31081 (*synth, cryst struct*)
Lazarini, F., *Acta Crystallogr., Sect. B*, 1977, **33**, 1954 (*cryst struct*)

IC-001473

$BiBr_6H_3$

Trihydrogen hexabromobismuthate(*III*)(3−), 9Cl

H_3BiBr_6

M 691.4
Salts synth. from $BiBr_3$ in HBr (aq.) + amine.
Tris-hydrazine salt: Yellow needles. V. sol. H_2O. Dec. at 215°.
Tris-$MeNH_2$ salt: [29532-34-1].
Pale yellow solid. Mp > 300°.
Tris-$EtNH_2$ salt: [29532-32-9].
Pale yellow solid. Mp 231-233°.
Tris-propylamine salt: [29532-31-8].
Pale yellow solid. Mp 254-255°.
Tris-Me_2NH salt: [19584-97-5].
Pale yellow cryst. (1-propanol/aq. HBr). Mp 264-266° (255°). Rhombohedral with two crystallographically independent cations and two anions. Interatomic distances: BiBr 284.9, 282.2 pm.
Tris-Et_2NH salt: [29718-11-4].
Pale yellow solid or cryst. (Me_2CO/2-propanol/HBr aq.). Mp 194-195°
Tris-diisopropylamine salt: [29532-29-4].
Pale yellow solid. Mp 230-232°.
Tris-Et_3N salt:
$C_{18}H_{45}BiBr_6N_3$ M 995.0
Rhombohedral: distorted $BiBr_6$ octahedra with three short Bi—Br (274.9 pm) and three long Bi—Br (300.6 pm) bonds in hexagonal unit cell.
Tris-aniline salt:
$C_{18}H_{18}BiBr_6N_3$ M 970.8
Cryst. + $2H_2O$. Mp 236°.

Pugh, W., *J. Chem. Soc.*, 1954, 1385 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 704 (*rev, bibl*)
Walton, R.A. *et al, Inorg. Chim. Acta*, 1967, **1**, 355 (*ae*)
McPherson, W.G. *et al, J. Phys. Chem.*, 1968, **72**, 3117 (*cryst struct*)
Walker, R.A., *Spectrochim. Acta, Part A*, 1968, **24**, 1527 (*ir, raman*)
Whealy, R.D. *et al, Inorg. Chim. Acta*, 1970, **4**, 420 (*synth*)
Hooper, H.A. *et al, Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)
Laane, J. *et al, Inorg. Chem.*, 1980, **19**, 44 (*ir, raman*)
Landers, A.G. *et al, Inorg. Chem.*, 1980, **19**, 744 (*Br-nqr*)

Lazarini, F., *Acta Crystallogr., Sect. C*, 1985, **41**, 1617 (*synth, cryst struct*)
Okuda, T. *et al, Z. Naturforsch., A*, 1986, **41**, 319 (*Br and Sb nqr*)

IC-001474

$BiBr_6Rb_3$

Trirubidium hexabromobismuthate(*III*)(3−), 9Cl
[21780-26-7]

$Rb_3[BiBr_6]$

M 944.8
Orthorhombic. Isolated octahedral anions with thoroughly irregular coordination polyhedra. Synth. from $Bi(OH)_3$ + Rb_2CO_3 + HBr aq. Yellow cryst. Mp *ca.* 530°. Dissoc. into RbBr and $BiBr_3$ at 530-585°.

Lazarini, F. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 2288 (*synth, cryst struct*)
Zalewicz, M. *et al, Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 1437 (*synth, props*)
Timmermans, C.W.M. *et al, Phys. Status Solidi B*, 1983, **118**, 353 (*props*)

IC-001475

BiClO

Bismuth chloride oxide (BiClO)
Chlorooxobismuthine, 9Cl. Chlorooxobismuth(III). *Bismuthyl chloride. Basic bismuth chloride. Bismuth oxychloride. C.I. Pigment white 14. C.I. Pigment white 31*
[7787-59-9]

BiClO

M 260.4
Tetragonal. Complex layer-lattice with Bi—O 231, Bi—Cl 307 pm. Alternate sheets of O and Cl atoms, with Bi atoms between. Each Bi is surrounded by 4 Cl's and 4O's with another Cl situated beyond centre of the large square face of the antiprism. Synth. from a basic bismuth nitrate and NaCl soln., or by diln. of conc. aq. $BiCl_3$ soln. Commercially available. Used in pigments, as artificial pearl. Formerly used in cosmetic preparations and as an antisyphilitic. Colourless fine powder or cryst. (platelets). V. sl. sol. H_2O; sol. dil. HCl, HNO_3. Mp 232°. Bp 447°. Sometimes known as Flake White, Bismuth White and Pearl White; these names also used for Bismuth nitrate oxide, IC-001515. In N_2, loses $BiCl_3$ at 570° to form, initially, $Bi_4O_5Cl_2$.
▷ EB2700000.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 689 (*rev, bibl*)
Ruimont, A., *Spectrochim. Acta, Part A*, 1972, **28**, 1287 (*ir*)
Morgan, W.E. *et al, Inorg. Chem.*, 1973, **12**, 953 (*pe*)
Davies, J.E.D., *J. Inorg. Nucl. Chem.*, 1973, **35**, 1531 (*ir, raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 598 (*synth*)
Bastow, T.J. *et al, J. Magn. Reson.*, 1977, **26**, 461 (*nqr*)
Segel, S.L., *J. Mol. Struct.*, 1980, **58**, 399 (*nqr*)
Nurgaliev, B.A. *et al, Zh. Neorg. Khim.*, 1985, **30**, 1665; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 948 (*synth*)
Taylor, P. *et al, Can. J. Chem.*, 1987, **65**, 2824 (*synth, props, cryst struct*)

IC-001476

BiClS

Bismuth chloride sulfide (BiClS), 9Cl, 8Cl
Chlorothioxobismuthine. Chlorothioxobismuth(III)
[19264-19-8]

ClBi=S

M 276.4
Each Bi is 7 coordinated by S (3×, at 260.5-271.1 pm) and Cl (4×, at 292.7-336.7 pm). One sulfur atom is at

the apex of a pyramid whose base is one of the S_2Cl_2 faces of a triangular prism formed by the Cl's and the two other sulfur atoms. The composite polyhedron is linked to others by shared pyramid S—S edges forming $(Bi_2Cl_8S_4)_n$ chains. Synth. from Bi_2S_3 + $BiCl_3$ at 300-350° and high press. Dark red (red-brown) needles. Mp 478°. Exists in paraelectric or ferroelectric states. Exhibits only low photosensitivity.

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1927, 168; *Suppl. Vol.*, 1964, 752 (*rev, bibl*)
Chepur, D.V. *et al, Phys. Status Solidi*, 1968, **30**, 461 (*ir*)
Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1969, **14**, 312 (*synth*)
Litvin, B.N. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 575; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 508 (*synth*)
Popolitov, V.I. *et al, Phys. Status Solidi A*, 1970, **3**, K1 (*synth*)
Furman, E. *et al, Phys. Rev. B: Solid State*, 1976, **13**, 1703 (*raman*)
Voutsas, G.P. *et al, Z. Kristallogr.*, 1980, **152**, 109 (*cryst struct*)

IC-001477

BiClSe

Bismuth chloride selenide (BiClSe), 8Cl
Chloroselenoxobismuthine. Chloroselenoxobismuth(III)
[24635-13-0]

ClBi=Se

M 323.3
Each Bi atom is coordinated by Se (3×; Bi—Se 272.7-285.5 pm) and Cl (3×; Bi—Cl 289.9-318.6 pm). Two Se and two Cl atoms form a parallelogram with remaining atoms as apices of pyramids based on the parallelogram. The coordination polyhedron is linked to symmetry-equivalent polyhedron by shared Se—Se edge forming $(Bi_2Se_4Cl_6)_n$ chains which are linked by common (Cl—Cl) chains. Synth. from $BiCl_3$ + Bi_2Se_3 at 360° *in vacuo* or in HCl at 350-530 atm. Dark red needles.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 771 (*rev, bibl*)
Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1969, **14**, 312 (*synth*)
Litvin, B.N. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 575; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 508 (*synth*)
Voutsas, G.P. *et al, Z. Kristallogr.*, 1986, **177**, 117 (*synth, cryst struct*)

IC-001478

$BiCl_3$

Bismuth(*III*) chloride ($BiCl_3$), 8Cl
Trichlorobismuthine, 9Cl. Trichlorobismuth(III)
[7787-60-2]

$BiCl_3$

M 315.3
Pyramidal geometry in vap. with Bi—Cl 248 pm; ClBiCl 100°. In cryst., distorted trigonal pyramidal (3 chlorines) with 5 additional Cl's forming a bicapped trigonal prism with Bi—Cl 246.5-252.8 pm, and 321.6-345.0 pm (bridging). Formed from Bi + Cl_2 or S_2Cl_2; or from Bi_2O_3 or $Bi(OH)_3$ + HCl. Catalyst in laboratory chemical reactions (e.g. Fries rearrangement, aldol reactions) and industrial processes (e.g. coal hydrocracking). White, deliquescent cryst. Insol. liq. NH_3; sl. sol. liq. SO_2, Me_2CO, HOAc. Mp 233°. Bp 447°, Bp 441°. V.p. 21.7 mm at 283°, 229 mm at 377°, 734 mm at 437°. Forms adducts with aromatic hydrocarbons, NH_3, SO_3, Et_2O, PCl_5, $POCl_3$, ketones. Combines with other metal chlorides (e.g. those of Group I) to give complex chlorides. ΔH_f° −379 kJ mol^{-1}.

Mesitylene complex (1:1): [18796-88-8]. *Trichloro(1,3,5-trimethylbenzene)bismuth*(III)
$C_9H_{12}BiCl_3$ M 435.5
Light yellow triclinic cryst. Mp 157° dec.
Hexamethylbenzene complex (2:1): [103349-18-4]. *Hexamethylbenzenebis[trichlorobismuth*(III)]
$C_{12}H_{18}Bi_2Cl_6$ M 792.9
Light yellow solid. Mp 212-215°.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 670 (*rev, bibl*)
Nyburg, S.C. *et al, Acta Crystallogr., Sect. B*, 1971, **27**, 2298; 1972, **28**, 2885 (*cryst struct*)
Denchik, E. *et al, J. Chem. Soc. A*, 1971, 3157 (*raman, props*)
Gillies, G.C. *et al, Can. J. Chem.*, 1972, **50**, 2586 (*nqr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 597 (*synth*)
Segal, S.L., *J. Mol. Struct.*, 1980, **58**, 399 (*nqr*)
Bartl, H., *Fresenius' Z. Anal. Chem.*, 1982, **312**, 17 (*cryst struct*)
Novak, I. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 635 (*pe*)
Schmidbaur, H. *et al, Chem. Ber.*, 1987, **120**, 1829, 1837 (*complexes*)
Mikov, S.N. *et al, Zh. Prikl. Spektrosk.*, 1987, **47**, 765; *Soviet J. Appl. Spectrosc.*, 1987, **47**, 140 (*raman*)
Haaland, A. *et al, Acta Chem. Scand., Ser. A*, 1988, **42**, 409 (*ed. struct*)

IC-001479

$BiCl_3NO_3^\ominus$

Trichloro(nitrato-*O*)bismuthate(*III*)(1−), 11Cl

$[BiCl_3(ONO_2)]^\ominus$

M 377.3 (ion)
K salt: [105012-41-7].
$BiCl_3KNO_3$ M 416.4
Synth. from Bi_2O_3 + HCl (aq.) + HNO_3 + KCl.
Colourless hexagonal cryst.

Davidovich, R.L. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1986, 1463; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1986, 1325 (*synth, cryst struct*)

IC-001480

$BiCl_3O_{12}$

Bismuth(*III*) perchlorate ($Bi(ClO_4)_3$)
Tri(perchlorato)bismuth(III)

$Bi(ClO_4)_3$

M 507.3
Synth. from $HClO_4$ aq. + Bismuth(*III*) hydroxide ($Bi(OH)_3$), IC-001503 or from $Bi(OOCCF_3)_3$ and $HClO_4$ aq. or Bi + $HClO_4$ aq. at < 100°. Cryst. in hydrated forms.
▷ Note explosive reaction between Bi and $HClO_4$ at > 110°.

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 693 (*rev, bibl*)
Kochegarov, V.M. *et al, Zh. Prikl. Khim. (Leningrad)*, 1964, **37**, 2323; *J. Appl. Chem. USSR (Engl. Transl.)*, 1964, **37**, 2296 (*synth, reactions*)

IC-001481

$BiCl_5H_2$

Dihydrogen pentachlorobismuthate(*III*)(2−)

$H_2[BiCl_5]$

M 388.2
Salts formed from $BiCl_3$ + amine.HCl in HCl aq.
Hydrogen hydrazine salt:
$BiCl_5H_4N_2$ M 420.3
Needles or plates + $2H_2O$.
Dihydrazine salt:
$BiCl_5H_8N_4$ M 452.3
Solid. Mp 190-195° dec.
Bis-$EtNH_3$ salt: [17525-26-7].

Long thin prisms. Mp 268°.
Bis-Me_2NH salt: Cryst. Mp 228°.
Bis-propylamine salt: Square leaflets. Mp 243°.
Bis-butylamine salt: [19439-83-9].
Sq. leaflets. Mp 225°.

Remy, H. *et al*, *Ber.*, 1928, **61**, 862 (*synth*)
Pugh, W., *J. Chem. Soc.*, 1954, 1385 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 686 (*rev, bibl*)
Oertel, R.P. *et al*, *Inorg. Chem.*, 1967, **6**, 1960 (*raman*)
Walton, R.A. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 355 (*ir*)
Walton, R.A. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 1527 (*ir, raman*)
Work, R.A. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 1547 (*ir, raman*)
Cariati, F. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 801 (*ir, raman*)

$BiCl_6Cs_2Na$ — IC-001482

Dicaesium sodium hexachlorobismuthate(3−), 9CI
Hexachlorobismuthate(III) *dicaesium sodium salt*
[27880-14-4]

$$Cs_2Na[BiCl_6]$$

M 710.4
Fcc struct. with Bi—Cl 267.6, Bi—Cs 469.1, Bi—Na 541.4 pm. Synth. from $BiCl_3$ + CsCl + NaCl heated in quartz ampoule at 850° or from $Bi^{3\oplus}$ + $Cs^{\oplus}$ + $Na^{\oplus}$ in 2*M* HCl. Yellowish single cryst.

Morss, L.R. *et al*, *Inorg. Chem.*, 1970, **9**, 1771 (*synth*)
Morss, L.R. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 653 (*cryst struct*)
Lynch, R.J. *et al*, *Adv. Nucl. Quadrupole Reson.*, 1974, **1**, 37 (*nqr, struct*)
Anistratov, A.T. *et al*, *Fiz. Tverd. Tela* (*Leningrad*), 1978, **20**, 3699; 1979, **21**, 2149; *Soviet Phys., Solid State* (*Engl. Transl.*), 1978, **20**, 2138; 1979, **21**, 1232 (*props*)
Smit, W.M.A. *et al*, *J. Phys. Chem. Solids*, 1980, **51**, 189.
Flerov, I.N. *et al*, *Ferroelectrics*, 1983, **48**, 97; 1985, **64**, 25 (*props*)
Pelle, F. *et al*, *Solid State Commun.*, 1984, **49**, 1089 (*synth, cryst struct, raman*)
Flerov, I.N. *et al*, *Fiz. Tverd. Tela* (*Leningrad*), 1987, **24**, 2267; *Soviet Physics. Solid State*, 1987, **24**, 1287 (*props*)

$BiCl_6H_3$ — IC-001483

Trihydrogen hexachlorobismuthate(*III*)(3−), 9CI, 8CI

$$H_3BiCl_6$$

M 424.7
Salts formed from $BiCl_3$ + amine + HCl aq.
Tris-$EtNH_2$ salt: [18756-47-3].
Cryst. Mp 239°.
Tris-Me_2NH salt: [50328-20-6].
Cryst. Mp 212°.
Tris-Me_3N salt: [43093-28-3].
Needles. Mp 272°.
Tris-Py salt: [34410-64-5].
$C_{15}H_{18}BiCl_6N_3$ M 662.0
Solid. Mp 234-236°.

[118144-86-8]

Remy, H. *et al*, *Ber.*, 1928, **61**, 862 (*synth*)
Pugh, W., *J. Chem. Soc.*, 1954, 1385 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 686 (*rev, bibl*)
Oertel, R.P. *et al*, *Inorg. Chem.*, 1967, **6**, 1960 (*raman*)
Walton, R.A. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 355 (*ir*)
Walton, R.A., *Spectrochim. Acta, Part A*, 1968, **24**, 1527 (*ir, raman*)
Paul, R.C. *et al*, *Indian J. Chem.*, 1971, **9**, 985 (*synth*)
Hooper, H.A. *et al*, *Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)
Work, R.A. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 1547 (*ir*)
Landers, A.G. *et al*, *Inorg. Chem.*, 1980, **19**, 744 (*synth, raman, struct*)
Du Bois, A. *et al*, *Z. Naturforsch., B*, 1988, **43**, 1003 (*synth, rev, bibl, cryst struct*)

$BiCl_6O_6P_3$ — IC-001484

Tris(phosphorodichloridato-*O*)bismuth, 9CI
Bismuth(III) *phosphorodichloridate*

$$Bi(O_2PCl_2)_3$$

M 610.6
$POCl_3$ complex: [41646-88-2].
$BiCl_9O_7P_4$ M 763.9
Synth. from $BiCl_3$ + Cl_2O in $POCl_3$. Insol. CCl_4. The O atoms of the dichlorophosphate ligands are arranged in pseudo-hexagonal manner around Bi.

Klopsch, A. *et al*, *Z. Naturforsch., B*, 1972, **27**, 1304 (*synth, ir, raman*)

$BiCuPbS_3$ — IC-001485

Aikinite
Bismuth copper lead sulfide (*$BiCuPbS_3$*)
[12232-84-7]

$$PbCuBiS_3$$

M 575.9
Bi has 3 and 5-fold coordination. Mineral, found in ores of Czechoslovakia, USSR, Greenland, Brazil and Europe. Black-grey metallic cryst.

Horiuchi, H. *et al*, *Can. Mineral.*, 1977, **15**, 527 (*cryst struct*)
Nakovicky, E. *et al*, *Can. Mineral.*, 1978, **16**, 405.
Kaplunnik, L.N. *et al*, *Deposited Doc.*, VINITI 92-82, 1981, 69 (*cryst struct*)
Friedrich, M., *Bel. Geowiss. Abh., Reihe A*, 1983, **46**, 109.

BiF — IC-001486

Bismuth(*I*) fluoride (BiF), 9CI
[13827-23-1]

$$BiF$$

M 227.9
Interatomic distance Bi—F 205.2 pm. Synth. from BiF_3 vap. on Bi(l) or from BiF_3 by electrical discharge in quartz tube. Disproportionates even at low temps. → Bi(s) + BiF_3(s).

Avasthi, M.N., *Spectrosc. Lett.*, 1970, **3**, 157.
Rai, B. *et al*, *Spectrosc. Lett.*, 1971, **4**, 129 (*bibl*)
Kuijpers, P. *et al*, *Chem. Phys.*, 1977, **24**, 97 (*formn, microwave*)
Chakoo, K.J. *et al*, *Indian J. Pure Appl. Phys.*, 1979, **17**, 189 (*formn, uv*)
Jones, W.E. *et al*, *J. Mol. Spectrosc.*, 1981, **90**, 481 (*uv*)
Ardashnikova, E.I. *et al*, *Zh. Neorg. Khim.*, 1987, **32**, 1796; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1987, **32**, 1067.

BiFO — IC-001487

Bismuth fluoride oxide (BiFO)
Fluorooxobismuthine, 9CI. Fluorooxobismuth(III). *Bismuthyl fluoride. Basic bismuth fluoride*
[13520-72-4]

$$BiFO$$

M 243.9

Tetragonal. Complex layer-lattice in which Bi is 9 coordinated with 4 oxygens and 4 fluorines forming a deformed square antiprism, and one fluorine is situated outside largest square face. Synth. from Bi_2O_3 + or from BiF_3 in sealed tube at 650°; or from $Bi(OH)_3$ + HF aq. with final dilution. White solid.
Mineral-form [24503-04-6]
Zavaritskite
Newly identified from Czechoslavkia.

Aurivillius, B., *Acta Chem. Scand.*, 1964, **18**, 1823 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 664 (*rev, bibl*)
Morrell, A. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 2502 (*formn*)
Rulmont, A., *Spectrochim. Acta, Part A*, 1972, **28**, 1287 (*synth, ir*)
Bastow, T.J. *et al*, *J. Magn. Reson.*, 1977, **26**, 461 (*synth, nqr*)

$BiFO_7Te_3$ — IC-001488

Bismuth fluoride tellurate, 9CI
[57572-07-3]

$$BiF(Te_3O_7)$$

M 722.7
α-phase is cubic. Synth. from Bi_2O_3 + BiF_3 + TeO_2 at 650°. Solid.

Meunier, G. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **281**, 367 (*synth, cryst struct*)

BiF_3 — IC-001489

Bismuth(*III*) fluoride (BiF_3)
Trifluorobismuthine, 9CI. Trifluorobismuth(III). *Bismuth trifluoride*
[7787-61-3]

$$BiF_3$$

M 265.9
Essentially an 8-coordinated struct. with some ionic character. Polymorphic. Synth. from $Bi(OH)_3$ or Bi_2O_3 + HF. Heavy white (grey when impure) cryst. powder. Insol. H_2O. Mp 725-730° (649°). Bp 900°. ΔH_f° −900 kJ mol^{-1}. Forms many complex halides with metal halides and hydrogen halides as well as with other halides of Group *V* elements.

α-form
Cubic. Should have coordination number 8, but this is decreased to 7 by displacement of Bi, and the fluorine polyhedron becomes a monocapped trigonal antiprism. At 200° converted into β-form.

β-form
Struct. comprises tricapped trigonal prism, with Bi coordinated by 9 fluorines, with Bi—F 221.7-250.2 (8 ×) and 310.0 (1 ×) pm.

γ-form
Orthorhombic with Bi—F 230.5-250.3 (8 ×) and 310.5 (1 ×) pm. Synth. from Bismuth chloride oxide (BiClO), IC-001475 + HF at 300°.

δ-form
Tetragonal. Synth. from γ-form by shock compression at *ca.* 5-7 × 10^3 atm. at 20°.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 659 (*rev, bibl*)
Cheetham, A.K. *et al*, *Acta Chem. Scand., Ser. A*, 1974, **28**, 55 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 218 (*synth*)
Poole, R.T. *et al*, *Phys. Rev. B. Solid State*, 1976, **13**, 896 (*pe*)
Greis, O. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **436**, 105 (*synth, cryst struct*)
Gely, J. *et al*, *J. Solid State Chem.*, 1982, **44**, 1 (*cryst struct, rev*)
Hovsk, I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 635 (*pe*)
Popov, A.I. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **576**, 242 (*reactions*)

BiF_4H_4N — IC-001490

Ammonium tetrafluorobismuthate

$$[NH_4^{\oplus}][BiF_4^{\ominus}]$$

M 303.0
Infinite layer struct. formed by edge- and face-sharing of polyhedra formed by the coordination of each Bi by nine F's. Interatomic distances: Bi—F 219-286 pm. Phys. props. not reported.

Aurivillius, B. *et al*, *Acta Chem. Scand.*, 1964, **18**, 1554 (*cryst struct*)

BiF_4K — IC-001491

Potassium tetrafluorobismuthate(*III*)(1−), 10CI
Bismuth potassium fluoride (*$BiKF_4$*)
[62389-76-8]

$$KBiF_4$$

M 324.0
Complex polymorphic system with α, β, β′, and γ phases recognised. Synth. from BiF_3 + KF at 280°. White solid. Forms a hexahydrate.

α-form
Low temp.-form
Synth. by annealing β-form at 250°. Equilibriates with β′-form.

β-form
Direct synth. (admixed with γ-form) from BiF_3. Also by annealing the γ-form at 25°. A fast ion conductor.

γ-form
By direct synthesis from BiF_3 when admixed with β-form.

[103223-04-7]

Lucat, C. *et al*, *J. Solid State Chem.*, 1979, **29**, 373 (*struct*)
Kalinchenko, F.V. *et al*, *Zh. Neorg. Khim.*, 1982, **27**, 2916; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 1653 (*synth*)
Matar, S. *et al*, *J. Solid State Chem.*, 1983, **50**, 1 (*synth*)
Zimina, G.V. *et al*, *Zh. Neorg. Khim.*, 1984, **29**, 1300; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1984, **29**, 745 (*synth, cryst struct*)
Matar, S.F. *et al*, *J. Phys. Chem. Solids*, 1988, **49**, 285 (*props, struct*)

BiF_4Na — IC-001492

Sodium tetrafluorobismuthate(1−), 10CI
Sodium bismuth(III) *tetrafluoride. Tetrafluorobismuthate*(III) (1−) *sodium salt*

$$NaBiF_4$$

M 307.9
Formed within a narrow homogeneity range. Synth. from NaF + BiF_3 at 450° in Pt crucible. A hydrate (3.5 H_2O) has been reported.

Fedorov, P.P. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2831; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1575 (*synth, cryst struct*)
Chartier, C. *et al*, *Mater. Res. Bull.*, 1981, **16**, 1159 (*formn, props*)
Novikova, E.N. *et al*, *Zh. Neorg. Khim.*, 1981, **26**, 774; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1981, **26**, 416 (*phase diagram*)
Kalichenko, F.V. *et al*, *Zh. Neorg. Khim.*, 1982, **27**, 2916; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 1653 (*phase diagram*)
Ikrami, D.D. *et al*, *C4*, 1986, **105**, 49884 (*synth, ir, struct*)

IC-001493

BiF_4Tl

Thallium(*I*) tetrafluorobismuthate(*III*)

[62389-78-0]

$Tl[BiF_4]$

M 489.3

Two forms: low temp. α-form isostructural with $PbCl_2$, and high temp. β-form has fluorite struct. Obt. from TLF + BiF_3 in liq. HF. Fluoride solid electrolyte.

▷ Highly toxic.

Lucat, C., *Mater. Res. Bull.*, 1977, **12**, 145.
Lucat, C. *et al*, *J. Solid State Chem.*, 1979, **29**, 373.

IC-001494

BiF_5

Bismuth fluoride (BiF_5), 9CI, 8CI

Bismuth(V) *pentafluoride. Pentafluorobismuth*(V)

[7787-62-4]

BiF_5

M 303.9

Polymeric tetragonal structure in solid with BiF_6 octahedra connected in infinite *trans*-chains with Bi—F 190 (4×), 211 (2×) pm. At least oligomeric in vap. Synth. from BiF_3 + F_2 at 500°. Powerful fluorinating agent. In combination with other fluorides e.g. K_2NiF_6, forms useful solid for the 'storage' and generation of F_2. Useful for removal of H_2O in HF preparations. Long white needles. V. sensitive to moisture. Sol. FSO_3H. Mp 154°. Bp 230°. Reacts with other metal fluorides e.g., under F_2 at 280° to give complex fluorides e.g. $MBiF_6$. Weaker Lewis acid than SbF_5.

▷ Highly toxic, mucous membrane irritant. Reacts explosively with H_2O, liberating O_3 and OF_2.

Beattie, I.R. *et al*, *J. Chem. Soc. A*, 1969, 958; 1971, 1910 (*ir, raman*)
Hebecker, C., *Z. Anorg. Allg. Chem.*, 1971, **384**, 111 (*cryst struct*)
Falconer, W.E. *et al*, *J. Fluorine Chem.*, 1974, **4**, 213 (*struct, ms*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 219 (*synth*)
Christe, K.O., *J. Fluorine Chem.*, 1978, **11**, 71 (*reactions, use*)
Kuz'min, A.I. *et al*, *Zh. Neorg. Khim.*, 1981, **26**, 821; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 440 (*nqr*)
Vopilov, V.A. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 625; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 350 (*F-19 nmr*)
Christe, K.O. *et al*, *Inorg. Chem.*, 1987, **26**, 2554 (*use*)
Popov, A.I. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **576**, 242 (*synth, ir, raman, reactions*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 523.

IC-001495

BiF_5K_2

Dipotassium pentafluorobismuthate(2−), 10CI

Dipotassium bismuth(III) *pentafluoride. Pentafluorobismuthate*(III) *dipotassium salt*

[84493-26-5]

K_2BiF_5

M 382.1

Cubic lattice. Tri- and hexa- hydrates have been characterised. Synth. from KF + BiF_3.

[103223-05-8, 103237-95-2]

Kalichenko, F.V. *et al*, *Zh. Neorg. Khim.*, 1982, **27**, 2916; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 1653 (*synth, cryst struct, phase diagram*)
Ikrami, D.D. *et al*, *CA*, 1986, **105**, 49884 (*synth, ir, cryst struct*)

IC-001496

BiF_6K

Potassium hexafluorobismuthate(*V*)(1−), 8CI

[26914-71-6]

$K[BiF_6]$

M 362.0

Synth. from KF + BiF_5 at 150°, or in Ni vessel under F_2 at 280°. Sl. sol. HF(l).

α-form

Cubic; interatomic distance: Bi—F 179 pm.

β-form

Tetragonal; interatomic distance: Bi—F 214-215 pm. By slow cooling of initial prep. in F_2 stream. Metastable form.

Fischer, J. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 6375 (*synth*)
Fukushima, E. *et al*, *J. Magn. Reson.*, 1969, **1**, 648 (*F-19 nmr*)
Fukushima, E., *J. Chem. Phys.*, 1971, **55**, 2463 (*F-19 nmr*)
Hebecker, C., *Z. Anorg. Allg. Chem.*, 1971, **384**, 12 (*synth, cryst struct*)
Christe, K.O. *et al*, *J. Fluorine Chem.*, 1978, **11**, 71 (*synth, raman*)
Popov, A.I. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **576**, 242 (*synth, ir, raman*)

IC-001497

$BiF_{10}Sb$

μ-Fluoropentafluoro(tetrafluoroantimony)bismuth, 11CI

Bismuth(V) *fluoride-antimony*(V) *fluoride adduct (1:1). Antimony bismuth fluoride* (*BiSbF*$_{10}$)

[95780-61-3]

$F_5BiFSbF_4$

M 520.7

Probably *trans*-bridged, covalent, polymeric or tetrameric struct. Synth. from BiF_5 + SbF_5 in WF_6.

Chen, G.S.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 9 (*synth, ir, raman, struct*)

IC-001498

$BiF_{15}Sb_2$

Antimony bismuth fluoride ($BiF_{15}Sb_2$), 11CI

Bismuth(V)*fluoride-antimony*(V)*fluoride adduct (1:2)*

[12232-91-6]

$BiF_5(SbF_5)_2$

M 737.4

Struct. thought to comprise 1:1 mixt. of $BiF_5(SbF_5)_3$ and $(BiF_2SbF_5)_2$ tetramers. See also Antimony bismuth fluoride ($BiF_{20}Sb_3$), IC-001499. Synth. from SbF_5 + BiF_5 in WF_6. Clear, colourless cryst. Mp 42-43°. Thermally stable up to 100°.

Chen, G.S.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 9 (*synth, ir, raman, ms, cryst struct, phase diagram*)

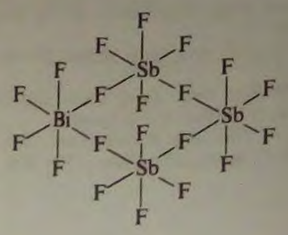
IC-001499

$BiF_{20}Sb_3$

Antimony bismuth fluoride ($BiF_{20}Sb_3$), 10CI

Tris(pentafluoroantimony)(pentafluorobismuth). Bismuth(V) *fluoride-antimony*(V)*fluoride adduct (1:3)*

[62046-99-5]



M 954.1

Formulated as $BiF_5(SbF_5)_3$. *Cis*-bridged struct. is analogous to that of SbF_5 in solid state. Synth. from BiF_5 + SbF_5 in WF_6. Well-defined, colourless cryst. Sol. WF_6. Mp 38-39°. Stable at 100° in sealed tube.

Chen, G.S.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 9 (*synth, ir, raman, ms, cryst struct, phase diagram*)

$BiHI_4$ IC-001500

Hydrogen tetraiodobismuthate(*III*)(1−), 9CI, 8CI

$H[BiI_4]$

M 717.6

Salts synth. from BiI_3 + amine + HI aq. Acid from BiI_3 and HI aq. Salts are sol. MeOH, MeCN, Me_2CO. Insol. C_6H_6, $CHCl_3$, CCl_4. Dilution of aq. solns. gives BiOI.

Tetrahydrate: Rhomb. pyramidal cryst.
Diisopropylamine salt: Deep red cryst. Mp 182-186°.
Tripropylamine salt: [19454-29-6].
Dark red cryst. (Me_2CO/HI aq.).
2-Methylpyridine salt: [18639-73-1].
Dark red cryst. (Me_2CO/HI aq.). Mp 199-201°.
Octahedral packing of iodines around two pairs of iodine bridges linking neighbouring Bi atoms results in infinite chain struct. Isomorphous with tetrabromo salt.

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1927, 159; 1964, 719 (*rev, bibl*)
Whealy, R.D. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 479 (*synth*)
Robertson, B.K. *et al*, *J. Phys. Chem.*, 1967, **71**, 3531 (*synth, cryst struct*)
Hooper, H.A. *et al*, *Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)
Laane, J. *et al*, *Inorg. Chem.*, 1980, **19**, 44 (*ir, raman*)
Nagapetyan, S.S. *et al*, *Zh. Neorg. Khim.*, 1989, **34**, 2244; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1989, **34**, 1276 (*synth, cryst struct*)

BiH_3 IC-001501

Bismuthine, 9CI, 8CI

Bismuth(III) *hydride. Bismuth trihydride*

[18288-22-7]

BiH_3

M 212.0

Well characterised as organic derivs. Synth. from $BiCl_3$ + $LiBH_4$ or $LiAlH_4$. Also by dec. (at −45°) of (di) methylbismuthine. Extremely unstable gas or liq. Mp −67°. Bp 16.8° (extrap.). ΔH_f° 277.8 kJ mol^{-1}. Ligand for Cr, Co, Fe, Mo and W.

▷ Presumed toxic.

Amberger, E., *Chem. Ber.*, 1961, **94**, 1447 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 626 (*rev, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 597 (*synth*)

BiH_3I_6 IC-001502

Trihydrogen hexaiodobismuthate(*III*)(3−), 8CI

$H_3[BiI_6]$

M 973.4

Discrete octahedral anion. Salts synth. from Bi_2O_3 in HI aq. + amine. Salts are sol. MeOH, DMF, MeCN, Me_2CO, less sol. EtOH. Insol. C_6H_6, $CHCl_3$, CCl_4. Dilution of aq. solns. gives BiOI.

Tris-hydrazine salt:
$BiH_{15}I_6N_6$ M 1069.5
Scarlet needles or tetragonal prisms. Mp 182° dec.

Tris-propylamine salt: [19478-43-4].
Orange-red cryst. Mp 265-267°.
Tris-diisopropylamine salt: [19478-44-5].
Orange-red cryst. Mp 211-213°.

Pugh, W., *J. Chem. Soc.*, 1954, 1385 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 718 (*rev, bibl*)
Whealy, R.D. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 479 (*synth*)
Laane, J. *et al*, *Inorg. Chem.*, 1980, **19**, 44 (*ir, raman*)

BiH_3O_3 IC-001503

Bismuth(*III*) hydroxide ($Bi(OH)_3$), 9CI, 8CI

Hydrobismuthic acid. Orthobismuthic acid. Bismuthic acid. Bismuth trihydroxide

[10361-43-0]

$Bi(OH)_3$

M 260.0

Has no acidic props. Synth. from $Bi^{3\oplus}$ aq. + NaOH aq., NH_4OH or $(NH_4)_2CO_3$. White to yellowish amorphous powder. Readily loses H_2O over H_2SO_4 *in vacuo*, or at 100-105°. V. sl. sol. H_2O. Sol. glycerol. Sol. acids → $Bi^{3\oplus}$. Reduced by HCHO → Bi metal. Adsorbent for U(*VI*).

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1927, 119 (*rev, bibl*)
Mambetov, A.A. *et al*, *Dokl. Akad. Nauk Azerb. SSR*, 1969, **25**, 20; *CA*, 1970, **73**, 38947 (*synth*)
Novosel, B. *et al*, *Colloid Polym. Sci.*, 1976, **254**, 409 (*synth*)
Podhodenko, V.N. *et al*, *Ukr. Khim. Zh. (Russ. Ed.)*, 1979, **45**, 496; *CA*, **91**, 101217 (*synth*)

$BiH_6O_6P_3S_6$ IC-001504

Tris(*O,O*-dihydrogen phosphorodithioato-*S,S'*)bismuth

$[(HO)_2P(S)S]_3Bi$

M 596.3

O,O,O',O',O'',O''-Hexaethyl ester: [21312-75-4]. *Tris*(O,O-*diethyl phosphorodithioato-S,S'*)*bismuth, 11CI*
$C_{12}H_{30}BiO_6P_3S_6$ M 764.6
Yellow cryst. Mp 55°.

O,O,O',O',O'',O''-Hexaisopropyl ester: [42294-79-1]. *Tris*[O,O-*bis(1-methylethyl)phosphorodithioato-S,S'*] *bismuth, 11CI*
$C_{18}H_{42}BiO_6P_3S_6$ M 848.8
Synth. from $BiCl_3$ + ammonium *O,O'*-diisopropylphosphorodithioate. Yellow prismatic cryst. (decane). Mp 67-68°. Monoclinic. Bi is 7-coordinate (including lone electron pair) in a trigonally distorted octahedron, with lone pair in one of the faces. Two groups of P—S bonds (200, 195 pm) and Bi—S bonds (270, 287 pm). Mean P—O (157.2 pm), C—O (150 pm) with OPO (100°) POC (124°), BiSP (85-90°), SPS (112°) and SPO (110, 112°).

Adams, D.M. *et al*, *J. Chem. Soc. A*, 1968, 1299 (*ir*)
Glidewell, C. *et al*, *Inorg. Chim. Acta*, 1971, **25**, 159 (*synth, P-31 nmr, struct*)
Lawton, S.L. *et al*, *Inorg. Chem.*, 1974, **13**, 135 (*synth, cryst struct*)
Chauhan, H.P.S. *et al*, *Phosphorus Sulfur*, 1983, **17**, 161 (*synth, pmr, P-31 nmr*)

$BiH_6O_6P_3Se_6$ IC-001505

Tris(dihydrogen phosphorodiselenato-*Se,Se'*)bismuth

$[(HO)_2P(Se)Se]_3Bi$

M 877.7

O,O,O',O',O'',O''-Hexaethyl ester: [26498-27-1]. *Tris*(O,O'-*diethyl phosphorodiselenato-Se,Se'*)*bismuth*
$C_{12}H_{30}BiO_6P_3Se_6$ M 1046.0

Orange cryst. (EtOH). Mp 113°.

Krishnan, V. *et al, Inorg. Chem.*, 1969, **8**, 2337 (*synth, ir, uv, cryst struct*)

IC-001506

BiI

Bismuth(*I*) iodide (BiI), 8CI

Iodobismuthylene, 9CI

[18933-08-9]

BiI

M 335.8

Detected in vap. over Bi—BiI_3 melts. Three modifications known. The α- and β- forms may be mixed valence compds. based on Bi_4I_4. Synth. by passing BiI_3 vap. over Bi(l) at 500°, or by dec. of BiI_3 at 700°, or from Bi + HgI_2. Black cryst.

α-form

Monoclinic. Characterised by 1D infinite chain of $[Bi_4I_4]$ units, with Bi atoms in two different environments. Interatomic distances: Bi—Bi 304.5, Bi—I 313.9 pm. Stable at <100°.

β-form

Monoclinic. Struct. generally as for α-form. Interatomic distances: Bi—Bi 304.5, Bi—I 313.5 pm. Obt. from the α-form at >100°.

γ-form

Monoclinic. Stable form at > *ca.* 290°. At *ca.* 310° dec. → BiI_3.

Cubicciotti, D., *J. Phys. Chem.*, 1961, **35**, 521 (*formn*)
Yamdagni, R., *Spectrochim. Acta, Part A*, 1970, **26**, 1071 (*uv*)
Trifonov, V.A. *et al, Zh. Neorg. Khim.*, 1975, **20**, 1470; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 825 (*synth*)
Kuijpers, P. *et al, Chem. Phys.*, 1976, **12**, 309 (*synth, microwave*)
von Schnering, H.G. *et al, Z. Anorg. Allg. Chem.*, 1978, **438**, 37 (*synth, cryst struct*)
Tischer, R. *et al, Chem. Phys.*, 1981, **62**, 115 (*microwave*)
Chervenyuk, G.I. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1982, **18**, 1827; *Inorg. Materials (Engl. Transl.)*, 1982, **18**, 1569 (*synth*)
Dikarev, E.V. *et al, Zh. Neorg. Khim.*, 1987, **32**, 430; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1987, **32**, 238 (*synth*)

IC-001507

BiIO

Bismuth iodide oxide (BiIO), 8CI

Iodooxobismuthine, 9CI. Iodooxobismuth(III). *Bismuthyl iodide. Basic bismuth iodide*

[7787-63-5]

BiIO

M 351.8

BiClO–type layer–lattice struct. Synth. from $Bi(NO_3)_3$ aq. + KI. Heavy, brick-red, odourless powder or copper-coloured cryst. Fuses at red-heat with part. dec. Insol. H_2O, $CHCl_3$. Sol. dil. aq. HCl. Mp 827° (incongr.). At 250-480° → Bi_5O_7I.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 722 (*rev, bibl*)
Shtilikha, M.V. *et al, Kristallografiya*, 1971, **16**, 840; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1971, **16**, 732 (*synth*)
Rulmont, A., *Spectrochim. Acta, Part A*, 1972, **28**, 1287 (*ir*)
Davies, J.E.D., *J. Inorg. Nucl. Chem.*, 1973, **35**, 1531 (*ir, raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 600 (*synth*)
Bastow, T.J. *et al, J. Magn. Reson.*, 1977, **26**, 461 (*nqr*)
Rulmont, A., *Rev. Chim. Minér.*, 1977, **14**, 277 (*synth, ir*)
Bordas, J. *et al, J. Phys. C*, 1978, **11**, 2607 (*uv*)
Taylor, P. *et al, Can. J. Chem.*, 1986, **64**, 290 (*synth, props*)

IC-001508

BiIS

Bismuth iodide sulfide (BiIS), 8CI

Iodothioxobismuthine, 9CI. Iodothioxobismuth(III)

[15060-32-9]

IBi=S

M 367.9

Orthorhombic. Synth. from BiI_3 + Bi_2S_3 at *ca.* 340°; or from Bi + S + I_2 at 540°; or from Bi + S + I_2 + H_2O, pH 6-7, 300-450°, high press. Black needles or platelets (red under microscope). Mp 535°. Ferroelectric or paraelectric. Exhibits photoelectric and electromechanical props. Exhibits phase changes at −40° and −158°. Loses BiI_3 when heated at 250° under N_2. Eventually leaves Bi_2S_3 at 450°.

Ryantsev, A.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1960, **6**, 1175; *Inorg. Materials (Engl. Transl.)*, 1960, **6**, 1025 (*phase diagram, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 753 (*rev, bibl*)
Chepur, D.V. *et al, Phys. Status Solidi*, 1968, **30**, 461 (*ir*)
Horak, J. *et al, Collect. Czech. Chem. Commun.*, 1969, **34**, 1475 (*props*)
Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; 1970, **15**, 1271; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1969, **14**, 312; 1970, **15**, 1118 (*synth*)
Semin, G.K., *Phys. Status Solidi A*, 1972, **11**, K61 (*nqr*)
Inorg. Synth., 1973, **14**, 160 (*synth*)
Teng, M.K. *et al, Phys. Status Solidi B*, 1974, **62**, 173 (*raman*)
Balkanski, M. *et al, Ferroelectrics*, 1977, **16**, 233 (*raman, props*)
Arivuoli, D. *et al, J. Mater. Sci.*, 1986, **21**, 2835 (*synth*)
Kumar, R.R. *et al, J. Mater. Sci.*, 1989, **24**, 4531 (*synth*)

IC-001509

BiISe

Bismuth iodide selenide (BiISe), 8CI

Iodoselenoxobismuthine, 9CI. Iodoselenoxobismuth(III)

[16035-71-5]

IBi=Se

M 414.8

Orthorhombic. Synth. from Bi + Se + I at 350-370° *in vacuo* or from Bi_2Se_3 + BiI_3 in HI at 300-400°/300-545 atm. Black needles or platelets. Mp 540° (congr.). Piezoresistant and ferroelectric. Exhibits marked photoelectric effect. Curie point 140°. Vap. readily dissociates. At 440-520° → BiI_3.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 772 (*rev, bibl*)
Horák, J. *et al, Krist. Tech.*, 1968, **3**, 231 (*synth, props*)
Chepur, D.V. *et al, Phys. Status Solidi*, 1968, **30**, 461 (*ir*)
Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1969, **14**, 312 (*synth*)
Popolitov, V.I. *et al, Phys. Status Solidi A*, 1970, **3**, K1 (*synth*)
Teng, M.K. *et al, Phys. Status Solidi B*, 1974, **62**, 173 (*raman*)
Arivuoli, D. *et al, J. Mater. Sci.*, 1987, **22**, 981 (*synth, props*)

IC-001510

BiITe

Bismuth iodide telluride (BiITe), 8CI

Iodotelluroxobismuthine, 9CI. Iodotelluroxobismuth(III)

[23309-61-7]

IBi=Te

M 463.4

Layer struct. Synth. from Bi + Te + I_2 at 480° *in vacuo*. Hexagonal lamellae. Mp 545° (470°)(congr.). Weak semiconductor. Unreactive to dil. aq. acid. Dec. by conc. HNO_3 and 1:1 HCl aq.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 818 (*rev, bibl*)

Chepur, D.V. *et al, Phys. Status Solidi*, 1968, **30**, 461 (*ir*)
Chepur, D.V. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 385; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 336 (*synth, cryst struct*)
Belotskii, D.B. *et al, Ukr. Khim. Zh. (Russ. Ed.)*, 1970, **36**, 897; *CA*, 1971, **74**, 57783 (*synth, phase diagram, props*)
Onopko, L.V. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, **10**, 1137; *Inorg. Materials (Engl. Transl.)*, 1974, **10**, 975 (*synth*)
Lošták, P. *et al, Phys. Status Solidi A*, 1980, **59**, 311 (*synth, optical props*)
Horak, J. *et al, Phys. Status Solidi A*, 1981, **63**, 407 (*electrical props*)

IC-001511

BiI_3

Bismuth(*III*) iodide (BiI_3)

Triiodobismuthine, 9CI. Triiodobismuth(III). *Bismuth triiodide*

[7787-64-6]

BiI_3

M 589.6

Rhombohedral. Hcp arrangement of iodine atoms with Bi atoms in the interstitial spaces. No discrete molecules. Synth. from Bi + I_2; or from $BiCl_3$ + SnI_4 or HI. Dark brownish violet hexagonal plates (CH_2I_2); also described as black or dark green. Forms reddish solns. in lower alcohols. Sl. sol. EtOH, C_6H_6. Insol. Et_2O. Mp 413° (407.7°). Bp 542° (extrap.), Bp 538°. Subl. under reduced press. ΔH_f° −150 kJ mol^{-1}. Readily forms complex halides with other metal iodides e.g. Disodium pentaiodobismuthate(2−), IC-001513.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 674 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 709 (*rev, bibl*)
Vashchenko, V.I., *Fiz. Tverd. Tela (Leningrad)*, 1967, **9**, 1577; *Soviet Physics: Solid State*, 1967, **9**, 1242 (*spectra*)
Belotski, D.B. *et al, Zh. Fiz. Khim.*, 1968, **42**, 1421; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1968, **42**, 740 (*optical props*)
Suri, S.K. *et al, Can. J. Chem.*, 1969, **42**, 3049 (*props, uv*)
Semin, G.K., *Phys. Status Solidi A*, 1972, **11**, K61 (*nqr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 600 (*synth*)
Schlüter, M. *et al, Phys. Status Solidi B*, 1976, **78**, 737 (*struct*)
Galy, J. *et al, J. Solid State Chem.*, 1982, **44**, 1 (*cryst struct, rev*)
Navak, I. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 635 (*pe*)
Wang, Y. *et al, J. Phys. Chem.*, 1987, **91**, 5005 (*uv*)

IC-001512

$BiI_4^\ominus$

Tetraiodobismuthate(*III*)(1−)

[14636-74-9]

$[BiI_4]^\ominus$

M 716.5 (ion)

Tbp struct. with electron lone pair eq.

Tetrabutylammonium salt: [22364-17-6]. Suggested for gravimetric or spectrophotometric detn. of Bi. Red cryst. Insol. H_2O; sol. $CHCl_3$. Mp 161-163°.

Ph_4As salt: [59890-68-5]. Suggested for spectrophotometric detn. of Bi. Orange-yellow solid. Insol. H_2O; sol. 1,2-dichloroethane.

H compd.: see *Hydrogen tetraiodobismuthate*(III)(1−), *IC-001500*

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 718 (*rev, bibl*)
Eve, A.J. *et al, Inorg. Chem.*, 1967, **6**, 331 (*uv*)
Spragg, R.A. *et al, J. Mol. Struct.*, 1969, **3**, 305 (*synth, struct*)
Ahlijah, G.Y. *et al, J. Chem. Soc. A*, 1970, 326 (*synth, ir, raman*)
Hasebe, K. *et al, Talanta*, 1982, **29**, 1135 (*uv*)
Burns, T.D. *et al, Anal. Chim. Acta*, 1987, **197**, 285; 1988, **211**, 305 (*anal*)

IC-001513

BiI_5Na_2

Disodium pentaiodobismuthate(2−), 8CI

Disodium bismuth(III) *pentaiodide. Pentaiodobismuthate*(III) *disodium salt*

Na_2BiI_5

M 889.4

Synth. from BiI_3 fused with NaI at 525°, or Bi_2O_3 + Na_2CO_3 + HI.

Tetrahydrate: [21028-86-4]. *Bismjol. Sodium iodobismuthite* $BiH_8I_5Na_2O_4$ M 961.5
Antisyphilitic. Odourless red cryst. with astringent taste. Hydrol. in soln. Sol. H_2O, EtOH, Me_2CO, EtOAc; sl. sol Et_2O. Mp 93° dec.

6.5 Hydrate: [75108-80-4].
Synth. from BiI_3 + NaI in EtOH aq. Bright red cryst. Darkens and dec. on drying over P_2O_5.

Bartczak, T. *et al, Zesz. Nauk Politech. Lodz. Chem.*, 1966, 15; *CA*, **69**, 31080 (*synth, cryst struct*)
Ziger, E.A. *et al, Zh. Neorg. Khim.*, 1980, **25**, 2168; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 1201 (*phase diagram, synth*)
Merck Index, 10th Ed., 1983, No. 1277 (*props*)
Dzeranova, K.B. *et al, Zh. Neorg. Khim.*, 1986, **31**, 1326; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1986, **31**, 756 (*phase diagram, synth*)
Griduneva, G.V. *et al, Zh. Neorg. Khim.*, 1988, **33**, 1718; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1988, **33**, 977 (*synth, cryst struct*)

IC-001514

$BiI_6^{3\ominus}$

Hexaiodobismuthate(*III*)(3−), 8CI

[14636-73-8]

$[BiI_6]^{3\ominus}$

M 970.4 (ion)

Tris-Me_4N salt: [19478-42-3].
Orange-red solid. Sol. MeOH, DMF, MeCN, Me_2CO; insol. C_6H_6, $CHCl_3$, CCl_4. Mp 310° dec. Dec. by H_2O.

H compd.: see *Trihydrogen hexaiodobismuthate*(III)(3−), *IC-001502*

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 718 (*rev, bibl*)
Whealy, R.D. *et al, Inorg. Chim. Acta*, 1967, **1**, 479 (*synth*)
Hooper, M.A. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 2335 (*raman*)
Spivakov, B.-Ya. *et al, J. Inorg. Nucl. Chem.*, 1979, **41**, 453 (*raman*)

IC-001515

$BiNO_4$

Bismuth nitrate oxide, 8CI

(Nitrooxy)oxobismuthine, 9CI. Bismuth oxynitrate. Bismuth subnitrate. Bismuth white. Pearl white. Spanish white. Basic bismuth nitrate

[10361-46-3]

$BiO(NO_3)$

M 286.9

Stated struct. now regarded as inaccurate. Several hydrates have revised structs. Commercially available. Pigment. Oxidiser.

Hemihydrate: see *Aquatetra-μ_3-hydroxy(nitrato-O)-tetra-μ_3-oxohexabismuth*(5+), *IC-001585*

Monohydrate: see *Tetra-μ_3-hydroxytetra-μ_3-oxohexabismuth*(6+), *IC-001584*

Sundvall, B., *Acta Chem. Scand., Ser. A*, 1979, **33**, 219.
Lazarini, F. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 448.

IC-001516

BiN_3O_9

Bismuth(*III*) nitrate

Bismuth trinitrate. Tris(nitrato-O,O')bismuth

[46140-16-3]

$Bi(NO_3)_3$

M 394.9

Isol. only as the pentahydrate which may be better formulated as the dihydrate of $[Bi(H_2O)_3(NO_3)_3]$.

Pentahydrate: Synth. from Bi, Bi_2O_3 or $Bi_2(CO_3)_3$ + HNO_3. Used in synth. of Bi salts, luminous paints. Commercially available. Oxidiser. Rgt. for cleavage of ethers. Hygroscopic lustrous colourless cryst. (HNO_3). Cannot be dehydrated. Mp 75°. Triclinic. Each Bi atom coordinated by 3 bidentate NO_3 groups, and also by 3 water molecules. Interatomic distances: Bi—O 225-297, Bi—OH_2 261-292 pm. Basic nitrates are formed when the pentahydrate is heated at 50-60°, or when an aq. soln. is diluted.

▷ Irritant.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 705 (*rev, bibl*)
Gattow, G. *et al, Z. Anorg. Allg. Chem.*, 1963, **324**, 31; 1965, **335**, 61 (*synth, ir, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 649 (*rev, bibl*)
Herpin, P. *et al, Bull. Soc. Fr. Minéral. Cristallogr.*, 1965, **88**, 590 (*cryst struct*)
Gattow, G. *et al, Naturwissenschaften*, 1967, **54**, 18 (*cryst struct*)
Oertel, R.P. *et al, Inorg. Chem.*, 1968, **7**, 1192 (*props, ir, raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 602 (*synth*)
Lazarini, F. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 1144 (*cryst struct*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 523 (*haz*)

IC-001517

$BiNaO_3$

Bismuth sodium oxide ($BiNaO_3$)

Sodium bismuthate(V) (*$NaBiO_3$*), *9CI*

[12232-99-4]

$NaBiO_3$

M 279.9

Ilmenite struct. Synth. from Bi_2O_3 + Na_2O_2, or from Na_2O + O_2. Powerful oxidant commercially available. Oxidises phenols; acyloins (→ α-diketones), and cleaves *vic*-diols. Oxidatively cleaves α-amino- and α-hydroxy-carboxylic acids. Used in inorg. analysis e.g. conversion of Mn to permanganate. Yellow to yellow-brown solid. Dec. at 400° → Na_2O + α-Bi_2O_3.

▷ VZ1750000.

Hydrate: Fine yellow needles. Variable water content, may be $2H_2O$, or $5H_2O$ but generally $3.5H_2O$. Dihydrate loses $1H_2O$ at 177°, and $1H_2O$ at 267°.

Gmelin Handbook Inorg. Chem., Syst. No. 21, *Suppl. Vol.*, 1928, 984; *Suppl. Vol.*, 1967, **4**, 1730 (*rev, bibl*)
Aurivillius, B., *Acta Chem. Scand.*, 1955, **9**, 1219 (*cryst struct*)
Miller, F.A. *et al, Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Dubovenko, L.I. *et al, Ukr. Khim. Zh. (Russ. Ed.)*, 1971, **37**, 1154; *CA*, 1972, **76**, 52381 (*ir*)
Morgan, W.E. *et al, Inorg. Chem.*, 1973, **12**, 953 (*pe*)
Goodenough, J.B. *et al, J. Solid State Chem.*, 1973, **9**, 493 (*struct*)
Adler, E. *et al, Acta Chem. Scand., Ser. B*, 1974, **28**, 883, 888 (*use*)
Kon, E. *et al, J. Org. Chem.*, 1975, **40**, 1515; 1976, **41**, 1646 (*use*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 604 (*synth*)
Wagner, C.D., *J. Electron Spectrosc. Relat. Phenom.*, 1977, **10**, 305 (*pe*)
Wagner, C.D. *et al, Anal. Chem.*, 1980, **52**, 1445 (*auger*)
Truesdale, L.K. *et al, J. Org. Chem.*, 1980, **45**, 726 (*use*)
Murashov, V.A. *et al, Zh. Neorg. Khim.*, 1985, **30**, 2966; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 1689 (*props, cryst struct*)
Tabeta, R. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3130C (*haz*)

IC-001518

BiO

Bismuth oxide (BiO), 9CI, 8CI

BiO

M 224.9

Polymeric-form [1332-64-5]

Obt. by dec. of Bi oxalate at 208° *in vacuo*. Black powder. In air, gives Bi_2O_3. Rhombohedrally distorted zinc blende struct. with both Bi and O exhibiting tetrahedral coordination. Bi—Bi bonds ⩾ 388; Bi—O 267-295 pm.

Dimeric-form [39326-72-2]

Bi_2O_2 M 449.9

Detected in Bi—O_2 system at *ca.* −250°. Believed to have planar 4-membered ring of Bi_2O_2.

Zav'yalova, A.A. *et al, Kristallografiya*, 1965, **10**, 480; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1965, **10**, 401 (*ed*)
Gadgil, L.H. *et al, Indian J. Chem.*, 1970, **8**, 431 (*synth*)
Zav'yalova, A.A. *et al, Zh. Strukt. Khim.*, 1972, **13**, 869; *J. Struct. Chem. USSR (Engl. Transl.)*, 1972, **13**, 811 (*cryst struct*)
Medernach, J.W. *et al, J. Am. Ceram. Soc.*, 1978, **61**, 494 (*rev*)
Sidorov, L.N. *et al, High Temp. Sci.*, 1980, **12**, 175 (*ms*)
Konnov, S.A. *et al, Zh. Fiz. Khim.*, 1981, **55**, 2893; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1981, **55**, 1645 (*ir, formn*)

IC-001519

BiO_2

Bismuth oxide (BiO_2)

Bismuth peroxide. Bismuth dioxide

[12048-50-9]

BiO_2

M 240.9

Thought to exist in two forms in Ar matrix at −250°. By reaction of Bismuth(*III*) nitrate, IC-001516 + peroxydisulfates, or by heating Bismuth oxide (Bi_2O_5), IC-001549 at 150-180°. Dark yellow, orange, ochre-yellow or yellow-brown solid.

Gattow, G. *et al, Z. Anorg. Allg. Chem.*, 1980, **470**, 25 (*synth*)
Konnov, S.A. *et al, Zh. Fiz. Khim.*, 1981, **55**, 2893; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1981, **55**, 1645 (*synth, ir*)
Begemann, B. *et al, J. Less-Common Met.*, 1989, **156**, 123 (*synth*)

IC-001520

BiO_4P

Bismuth phosphate ($BiPO_4$)

[10049-01-1]

$BiPO_4$

M 303.9

Synth. from Bi_2O_3 + P_2O_5 or $NaPO_3$ at melt, or from $Bi(NO_3)_3$ + H_3PO_4 or Na_3PO_4. Has been employed in extraction of plutonium. Known with monazite-type struct. (stable over wide temp. range); a monoclinic high temp. form which slowly converts at r.t. into the monazite-type.

Mooney-Slater, R.C.L., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1962, **117**, 371 (*cryst struct*)
Chudinova, N.N., *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1973, **11**, 1662; *Inorg. Materials (Engl. Transl.)*, 1973, **11**, 1422 (*pe*)
Lepin, Y.K. *et al, CA*, 1974, **80**, 140848 (*synth*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 603 (*synth*)
Obrubov, V.A. *et al, Zh. Prikl. Khim. (Leningrad)*, 1980, **53**, 256; *J. Appl. Chem. USSR (Engl. Transl.)*, 1980, **53**, 197 (*synth*)
Watanabe, M. *et al, CA*, 1986, **105**, 10613 (*synth*)

IC-001521

BiO_4Sb

Antimony bismuth oxide ($SbBiO_4$), 10CI

Bismuth orthostibate

[22633-00-7]

$SbBiO_4$

M 394.7

Monoclinic. Synth. from Bi_2O_3 + Sb_2O_5 aq. followed by dehydration at 140-280° and fusion at 1250-1305°. Yellowish powder or elongated rod-like cryst. Highly birefringent. Mp *ca.* 1305°.

Nedil'ko, S.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1976, **12**, 2014; *Inorg. Materials (Engl. Transl.)*, 1976, **12**, 1652 (*synth, cryst struct*)
Kochetkov, V.V. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1981, **17**, 842; *Inorg. Materials (Engl. Transl.)*, 1981, **17**, 587 (*struct*)
Rakhmatova, Z.M. *et al, Khim. Tverd. Tela*, 1984, **7**, 72; *CA*, **104**, 195797 (*synth, ir, raman*)

IC-001522

BiO_6Re_2

Bismuth rhenium oxide ($BiRe_2O_6$), 10CI

[73079-49-9]

$BiRe_2O_6$

M 677.3

Mixed valency compd. Re(*IV*)-(*V*). Struct. has Re_2O_{10} unit with Re-Re 240 to 250 pm. Synth. from ReO_3 and Bi_2O_3.

Rae-Smith, A.K. *et al, J. Solid State Chem.*, 1979, **30**, 345.
Cheetham, A.K. *et al, Mater. Res. Bull.*, 1981, **16**, 7 (*synth, struct, props*)

IC-001523

$BiPS_4$

Bismuth(3+) phosphorotetrathioate, 9CI

Bismuth(III) *tetrathiophosphate. Bismuth thiophosphate. Phosphorotetrathioic acid, Bi(3+) salt (1:1)*

[30009-57-5]

$BiPS_4$

M 368.2

Synth. from Bi + S + P/I_2. Orthorhombic. Network of S tetrahedra every second of which is occupied by a P atom. S-tetrahedra share edges in parallel chains. 6 or 8-coordination around Bi and S. Bi—S 268-330, P—S 200-208 pm, SPS 104.9-115.6°. Dark red prisms with metallic grey lustre, or red powder. Electrically conducting. In N_2 at 450° gives Bi_2S_3 + $'P_2S_5'$. In O_2 at 400-800°, gives $BiPO_4$.

Nitsche, R. *et al, Mater. Res. Bull.*, 1970, **5**, 419 (*synth*)
Zimmermann, H. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2003 (*synth, cryst struct*)
Schulte-Kellinghaus, M. *et al, Thermochim. Acta*, 1978, **27**, 141 (*synth, props*)
Dordyai, V.S. *et al, Zh. Neorg. Khim.*, 1979, **24**, 2886; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1603 (*ir, struct*)
Elhaidouri, A. *et al, Rev. Chim. Minér.*, 1986, **23**, 138 (*synth, props*)

IC-001524

$BiPSe_4$

Bismuth(3+) phosphorotetraselenate, 9CI

Bismuth(III) *tetraselenophosphate. Bismuth selenophosphate*

[54421-86-2]

$BiPSe_4$

M 555.7

Obt. from P_2Se_5 + Bi_2Se_3 at 700°. Black cryst. Dec. into precursors at 400-500°.

Brusilovets, A.I. *et al, Zh. Neorg. Khim.*, 1974, **19**, 3167; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 1732.

IC-001525

BiS

Bismuth sulfide (BiS), 9CI

[12048-34-9]

BiS

M 241.0

Struct. unknown, but may be $Bi^{3\oplus}(BiS_4)^{3\ominus}$. Synth. from Bi + S. Grey needles.

Cubicciotti, D., *J. Phys. Chem.*, 1963, **67**, 118, 1385 (*phase diagram, ms*)
Barrow, R.F. *et al, Proc. Phys. Soc., London*, 1967, **90**, 555 (*uv*)
Uy, O.M. *et al, Trans. Faraday Soc.*, 1969, **65**, 3221 (*formn, ms*)

IC-001526

BiSb

Bismuth antimonide (BiSb), 9CI, 8CI

Antimony compd. with Bi (1:1), 10CI

[12323-19-2]

BiSb

M 330.7

Synth. from Bi + Sb at melt. Semiconductive alloy. Commercially available. Cryst. Mp 475°.

Kohl, F.J. *et al, J. Am. Chem. Soc.*, 1967, **89**, 5501; 1968, **90**, 4814 (*ms*)
Vezzoli, G.C., *Mater. Res. Bull.*, 1986, **21**, 315 (*electrical props*)

IC-001527

$BiSbTe_3$

Antimony bismuth telluride

Bismuth antimony telluride

[12589-80-9]

$(Bi,Sb)_2Te_3$

M 713.5

A solid soln. of Sb_2Te_3 and Bi_2Te_3. Used in solar cells. Thermoelectric material (*p*-type).

Airapetyants, S.V. *et al, Sov. Phys.-Tech. Phys.*, 1958, **3**, 1632 (*thermoelectricity*)
Smith, M.J. *et al, J. Appl. Phys.*, 1962, **33**, 2186 (*phase diagram*)
Bekebrede, W.R. *et al, Phys. Chem. Solids*, 1962, **23**, 1023 (*cryst struct*)

IC-001528

BiSe

Bismuth selenide (BiSe), 9CI, 8CI

[12010-54-7]

BiSe

M 287.9

Layered system with hexagonal struct. Synth. from Bi + Se at 750° *in vacuo*; from Bi + PbSe; by dissociation of Bi_2Se_3. Plates. Dissociation energy 276.5 kJ mol^{-1}.

Stasova, M.M., *Zh. Strukt. Khim.*, 1967, **8**, 655; *J. Struct. Chem. USSR (Engl. Transl.), Engl. Transl.*, 1967, **8**, 584 (*cryst struct*)

Uy, O.M. *et al*, *Trans. Faraday Soc.*, 1969, **65**, 3221 (*formn, ms*)
Abukosov, N.Kh. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 1401; *Inorg. Materials (Engl. Transl.)*, 1972, **8**, 1237 (*synth, props*)
Dumon, A. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1973, **70**, 1546 (*phase diagram, formn*)
Boechko, V.F. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1975, **11**, 551; *Inorg. Materials (Engl. Transl.)*, 1975, **11**, 469 (*synth, struct*)
Gardes, B. *et al*, *Eur. J. Solid State Inorg. Chem.*, 1989, **26**, 221 (*cryst struct*)

IC-001529

BiTe

Bismuth telluride (BiTe), 9CI, 8CI

[12010-57-0]

BiTe

M 336.5
Polymeric struct. based on cubic packing with layers.
Synth. from Bi + Te at 800°; or from Bi + PbTe.
Dissociation energy 228.5 kJ mol^{-1}.

Mineral-form [69257-36-9]
Tsumoite
Found at site near Hiroshima in Japan. Trigonal silver-white metallic cryst.

Uy, O.M. *et al*, *Trans. Faraday Soc.*, 1969, **65**, 3221 (*formn, ms*)
Abukosov, N.Kh. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 1401; *Inorg. Materials (Engl. Transl.)*, 1972, **8**, 1237 (*synth, props*)
Zhukova, T.B. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1976, **12**, 539; *Inorg. Materials (Engl. Transl.)*, 1976, **12**, 467 (*struct*)
Yamana, K. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 147 (*synth, cryst struct*)

IC-001530

[BiTh]

Thorium bismuth
Bismuth thorium

Thorium bismuthide (***Th_2Bi***) [77681-57-3]
$BiTh_2$ M 673.0
Studied as heat transfer agent for nuclear reactors, and for sepn. of rare earths from Bi. ΔH_f −62.7 kJ mol^{-1}.

Thorium bismuthide (***Th_5Bi_3***) [83619-19-6]
Bi_3Th_5 M 1787.1
Isostructural with Mn_5Si_3. ΔH_f −63 kJ mol^{-1}.

Thorium bismuthide (***ThBi***) [12409-35-7]
BiTh M 441.0
NaCl struct. ΔH_f −81.1 kJ mol^{-1}.

Thorium bismuthide (***Th_3Bi_4***) [12409-51-7]
Bi_4Th_3 M 1532.0
Isostructural with Th_3P_4. ΔH_f −79.4 kJ mol^{-1}.

Thorium bismuthide (***$ThBi_2$***) [12409-39-1]
Bi_2Th M 649.9
Isostructural with Cu_2Sb, UBi_2, $ThAs_2$ $ThSb_2$. ΔH_f −69 kJ mol^{-1}.

Ferro, R., *Acta Crystallogr.*, 1957, **10**, 476 (*cryst struct, $ThBi_2$*)
Hulliger, F., *J. Less-Common Met.*, 1968, **16**, 113.
Dahlke, V. *et al*, *Z. Metallk.*, 1969, **60**, 465 (*$ThBi_2$*)
McNeese, L.E., *U.S. At. Energy Comm.*, 1970, URNL-TM-3053; *CA*, **75**, 75651 (*use*)
Poyarkov, A.M. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, 118 (*thermodyn*)
Borsese, A. *et al*, *J. Less-Common Met.*, 1980, **70**, 213 (*thermodyn*)
Borzone, G. *et al*, *J. Less-Common Met.*, 1982, **84**, 165 (*cryst struct*)

IC-001531

[BiTl]

Thallium bismuthide

Thallium bismuthide (***$TlBi_2$***) [12048-58-7]
Bi_2Tl M 622.3
Homogeneous phase in the Bi—Tl system.

Olander, A., *Z. Physik. Chem., Abt. A*, 1934, **169**, 260 (*formn*)
Robinson, P.M. *et al*, *Trans. Am. Inst. Min., Metall. Pet. Eng.*, 1965, **233**, 1908 (*thermodyn*)

IC-001532

[BiU]

Uranium bismuthides
Uranium bismuth. Bismuth uranium

▷ All phases are unstable in air and pyrophoric.

Uranium bismuthide (***UBi***)
BiU M 447.0
NaCl struct. Antiferromagnetic below 285-290K.

Uranium bismuthide (***U_3Bi_4***)
Bi_4U_3 M 1550.0
Th_3P_4 struct. T_c 108-112K. μ_{eff} = 3.1-3.14μ_B (θ 110-111°) (<300K).

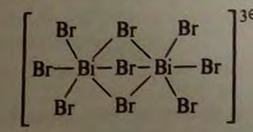
Uranium bismuthide (***UBi_2***)
Bi_2U M 655.9
Cu_2Sb struct. Antiferromagnetic transition at 180-194K. μ_{eff} = 2.10μ_B (80K).

Ferro, R., *Atti R. Accad. Naz. Lincei, Rend. Cl. Sci. Fis., Mat. Nat.*, 1952, **13**, 401 (*synth, struct*)
Trzebiatowski, W. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1966, **14**, 495 (*struct*)
Kuznietz, M. *et al*, *J. Phys. Chem. Solids*, 1969, **30**, 1642.
Sternberk, J. *et al*, *J. Phys. (Paris)*, Suppl. 1, 1971, **32**, C1-744, C1-745 (*magnetism*)
Troć, R. *et al*, *Phys. Status Solidi B*, 1971, **43**, 147 (*magnetism, UBi*)
Pauliikowski, A. *et al*, *J. Phys. C*, 1979, **12**, 2373 (*magnetism, UBi*)
Mallett, C.P. *et al*, *Phys. Status Solidi B*, 1979, **94**, 257 (*magnetism, UBi*)
Gmelin Handbook Inorg. Chem., Syst. No. 55, *Suppl.*, 1981, C14, 2281 (*rev*)

IC-001533

$Bi_2Br_9^{3\ominus}$

Tri-μ-bromohexabromodibismuthate(3−), 8CI
Nonabromodibismuthate(III)(*3*−)



M 1137.0 (ion)

Tris-Me_4N salt: [15809-67-3].
$C_{12}H_{36}Bi_2Br_9N_3$ M 1359.5
Synth. from Me_4NBr + $BiBr_3$ in HBr(aq.). Hexagonal air-stable yellow cryst. Anions consist of face-sharing $BiBr_6$ octahedra. Interatomic distances: Bi—Br_{br} 306; Bi—Br_{term} 272 pm; angle: $BiBrBi_{br}$ 82.5°.

Tris-Et_4N salt: [30335-20-7].
Synth. from $[Et_4N]Br$ + $BiBr_3$ in HBr aq. Solid. Dec. at 295°.

Tris-Ph_4P salt: [64164-19-8].
Synth. from $[Ph_4P]Br$ + $BiBr_3$ in Me_2CO. Solid. Monoclinic. Molecular dimensions: irregular anion with face-sharing $BiBr_6$ octahedra Br—Br_{br} 299.4-311.5, Bi—Br_{term} 271.0-277.3 pm.

Tri-Cs salt: see *Tricaesium tri-μ-bromohexabromodibismuthate*(III)(*3*−), *IC-001534*

Tri-H compd.: see *Trihydrogen tri-μ-bromohexabromodibismuthate*(III)(*3*−), *IC-001535*

Preer, J.R. *et al*, *Inorg. Chem.*, 1966, **5**, 656 (*synth*)

Whealy, R.D. *et al*, *Inorg. Chim. Acta*, 1970, **4**, 420 (*synth*)
Work, R.A. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 1547 (*ir, uv*)
Lazarini, F., *Acta Crystallogr., Sect. B*, 1977, **33**, 2686 (*synth, cryst struct*)
Lazarini, F., *Cryst. Struct. Commun.*, 1980, **9**, 815 (*synth, cryst struct*)
Landers, A.G. *et al*, *Inorg. Chem.*, 1980, **19**, 744 (*synth, nqr, struct*)
Zaleski, J. *et al*, *Z. Naturforsch., A*, 1989, **44**, 1102 (*props*)

IC-001534

$Bi_2Br_9Cs_3$

Tricaesium tri-μ-bromohexabromodibismuthate(*III*)(3−), 9CI
Caesium nonabromodibismuthate
[12233-16-8]

$Cs_3[Bi_2Br_9]$

M 1535.8
Trigonal. Cs—Br close packed. $BiBr_6$ octahedra share three *cis*-vertices with three other octahedra forming corrugated layers. Synth. from Cs_2CO_3 + Bismuth(*III*) hydroxide ($Bi(OH)_3$), IC-001503 in HBr aq. or from $BiBr_3$ + CsBr in H_2O. Provides a means of separating Cs from Na, K or Rb. Yellow cryst. Insol. H_2O.

Gmelin Handbook Inorg. Chem., Syst. No. 25, 1938, 251 (*rev, bibl*)
Plyushchev, V.E. *et al*, *Zh. Prikl. Khim. (Leningrad)*, 1975, **48**, 637; *J. Appl. Chem. USSR (Engl. Transl.)*, 1975, **48**, 653 (*synth, use*)
Lazarini, F., *Acta Crystallogr., Sect. B*, 1977, **33**, 2961 (*synth, cryst struct*)
Zalewicz, M. *et al*, *Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 1437 (*props*)
Timmermans, C.W.M. *et al*, *Phys. Status Solidi B*, 1981, **106**, 647; 1983, **115**, 267 (*props*)

IC-001535

$Bi_2Br_9H_3$

Trihydrogen tri-μ-bromohexabromodibismuthate(*III*)(3−), 8CI
Trihydrogen nonabromodibismuthate

$H_3[Bi_2Br_9]$

M 1140.1
Salts synth. from $BiBr_3$ in HBr aq. and amine.

Tris-hydrazine salt:
$Bi_2Br_9H_{15}N_6$ M 1236.2
Yellow needles or prisms.

Tris-$MeNH_2$ salt: [72318-18-4].
Exists in paraelectric, pyroelectric, or ferroelectric phases, with transitions at 188K, 140K and 101.5K.

Tris-Et_3N salt: [30815-45-3].
Pale yellow solid. Mp 102-104°.

Tris-diisobutylamine salt: [29532-24-9].
Pale yellow solid. Mp 161-162°.

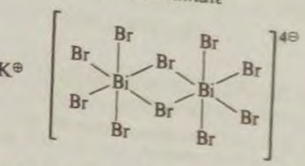
Tris-piperidine salt: [69853-25-4].
Yellow solid. Insol. polar solvs. Stable in air.

Pugh, W., *J. Chem. Soc.*, 1954, 1385 (*synth*)
Whealy, R.D. *et al*, *Inorg. Chim. Acta*, 1970, **4**, 420 (*synth*)
Cariati, F. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 801 (*synth, ir, raman*)
Laane, J. *et al*, *Inorg. Chem.*, 1980, **19**, 44 (*ir, raman*)
Landers, A.G. *et al*, *Inorg. Chem.*, 1980, **19**, 744 (*synth, raman, struct*)
Jakubas, R. *et al*, *Ferroelectrics*, 1988, **77**, 129 (*synth, props*)
Kozul, P. *et al*, *Solid State Commun.*, 1989, **72**, 143 (*props*)

IC-001536

$Bi_2Br_{10}K_4$

Tetrapotassium di-μ-bromooctabromodibismuthate(*III*), 11CI
Tetrapotassium decabromodibismuthate



M 1373.3
Two $BiBr_6$ octahedra sharing common edge.
Tetrahydrate: [63372-87-2].
Synth. from $Bi(OH)_3$ + K_2CO_3 in HBr aq.
Orthorhombic. Isomorphous with tetraammonium salt tetrahydrate. Shows blue luminescence at low temps.

Lazarini, F., *Acta Crystallogr., Sect. B*, 1977, **33**, 1954 (*synth, cryst struct*)
Timmermans, C.W.M. *et al*, *Phys. Status Solidi B*, 1983, **118**, 353 (*props*)

IC-001537

$Bi_2Cs_3I_9$

Tricaesium tri-μ-iodohexaiodobismuthate(*III*)(3−), 9CI
Caesium nonaiodobismuthate(III)
[23351-26-0]

$Cs_3[Bi_2I_9]$

M 1958.8
Hexagonal. Hexacoordinated bismuth atoms in confacial octahedra. Close packing of Cs and I atoms.
Interatomic distances: Bi—I_{term} 292.3, Bi—I_{br} 324.9 pm.
Synth. from CsI + BiI_3 + HI aq., or $CsNO_3$ soln. diffused into NaI + Bi_2O_3 in HOAc. Provides a means of detecting and determining Cs in the presence of K or Rb. Red-brown bipyramidal cryst. (HI aq.). Mp 632° (incongr.). Stable in air to *ca.* 490°, then dec. to CsI + BiI_3.

Gmelin Handbook Inorg. Chem., Syst. No. 25, 1938, 251 (*rev, bibl*)
Lindqvist, O., *Acta Chem. Scand.*, 1968, **22**, 2943 (*synth, cryst struct*)
Savel'eva, L.V. *et al*, *Zh. Neorg. Khim.*, 1972, **17**, 1485; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1972, **17**, 769 (*synth*)
Chabot, B. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 645 (*cryst struct*)
Zalewicz, M. *et al*, *Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 1437 (*synth, props*)
Kun, S.V. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1988, **24**, 1899; *Inorg. Materials (Engl. Transl.)*, 1988, **24**, 1622 (*phase diagram*)

IC-001538

Bi_2FNbO_5

Bismuth(*III*) niobium(*V*) fluoride oxide (Bi_2NbFO_5), 11CI
[60861-74-7]

Bi_2NbFO_5

M 609.8
Struct. contains layers of composition $Nb(O,F)_4$ formed by corner-shared octahedra. Synth. hydrothermally from Bi_2O_3, BiF_3 and Nb_2O_5 in aq. NH_4F. The synth. by Aurivillius yields an impure product.

Aurivillius, S., *Ark. Kemi.*, 1952, **4**, 39 (*cryst struct*)
Kodama, H. *et al*, *J. Solid State Chem.*, 1981, **36**, 349 (*synth*)

$Bi_2H_2O_7S$ IC-001539

μ-Hydroxyhydroxy-μ-oxo[sulfato(2−)-*O*]dibismuth, 11CI

Basic bismuth sulfate monohydrate

[84576-62-5]

$[Bi_2O(OH)_2]SO_4$

M 564.0

Previously formulated as $(BiO)_2SO_4.H_2O$. Monoclinic. Bi atoms coordinated irregularly. Cryst.

Aurivillius, B., *Acta Chem. Scand.*, 1964, **18**, 2375 (*cryst struct*)
Golič, L. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2881 (*synth, cryst struct*)

$Bi_2H_3I_9$ IC-001540

Trihydrogen tri-μ-iodohexaiododibismuthate(*III*)(3−)

Trihydrogen nonaiododibismuthate(III)

$H_3[Bi_2I_9]$

M 1563.1

Salts from BiI_3 + amine + HI (aq.). Salts are sol. MeOH, DMF, MeCN, Me_2CO, less sol. EtOH. Insol. C_6H_6, $CHCl_3$, CCl_4. Diln. of aq. solns. of salts gives BiOI.

Tris-$MeNH_2$ salt: Red solid. Mp 300° dec.

Tris-Me_2NH salt: [12327-10-5].
Red solid. Mp 306° dec.

Tris-Et_2NH salt: [12327-43-4].
Red cryst. Anion consists of face-sharing octahedra with Bi—I (terminal) 293.4-303.2 Bi—I (bridge) 316.9-327.7 pm.

Tris-Et_3N salt: Mp 133-135°.

Tris-aniline salt: Red solid. Mp 171-175°.

Tris(4-methylpyridine) salt: [12327-81-0].
Mp 203-205°.

Whealy, R.D. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 479 (*synth*)
Cariati, F. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 801 (*synth, ir, raman*)
Laane, J. *et al*, *Inorg. Chem.*, 1980, **19**, 44 (*ir, raman*)
Lazarini, F., *Acta Crystallogr., Sect. C*, 1987, **43**, 875 (*cryst struct*)
Gridunova, G.V. *et al*, *Zh. Neorg. Khim.*, 1988, **33**, 1718; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1988, **33**, 977 (*synth, cryst struct*)

Bi_2H_4 IC-001541

Dibismuthine, 9CI

[21972-71-4]

Bi_2H_4

M 421.9

Too unstable to be isolable. Many organic derivs. known. Complexes with $W(CO)_5$.

Arif, A.M. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 1062.
Arif, A.M. *et al*, *Inorg. Chem.*, 1986, **25**, 4836.

$Bi_2H_6O_{12}S_3$ IC-001542

Diaquadi-μ-hydroxybis[sulfato(2−)-*O*]dibismuth, 11CI

Di-μ-hydroxobis[aquasulfatobismuth(III)*]. Bismuth hydroxide sulfate monohydrate*

[83896-75-7]

$Bi_2(H_2O)_2(SO_4)_2(OH)_2$

M 680.1

Usually formulated as $BiOH.SO_4.H_2O$ or $Bi_2O_2.2Bi_2(SO_4)_3.9H_2O$. Monoclinic. Struct. contains the rhomboidal, planar $[Bi_2(OH)_2]^{4\oplus}$ ion. One $SO_4^{2\ominus}$ oxygen and one H_2O are bonded to each Bi quite strongly. Coordination around each Bi completed from O atoms of other SO_4 groups at longer distances. The coordination polyhedra are distorted octahedra. Synth. by slow diffusion of H_2O into acid-sat. soln. of Bismuth(*III*) sulfate ($Bi_2(SO_4)_3$), IC-001556. First product of hydrol. of bismuth sulfate.

'Monomeric' formulation: Bismuth hydroxide sulfate monohydrate

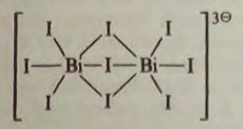
BiH_3O_6S M 340.0

Margulis, E.V. *et al*, *Zh. Neorg. Khim.*, 1965, **10**, 2304; 1967, **12**, 2036; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 1253; 1967, **12**, 1072 (*synth*)
Graunar, M. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2879 (*synth, cryst struct*)

$Bi_2I_9^{3\ominus}$ IC-001543

Tri-μ-iodohexaiododibismuthate(*III*)(3−), 8CI

Nonaiododibismuthate(3−)



M 1560.1 (ion)

Tris-Me_4N salt: [75009-60-8].
Synth. from Me_4NBr + $BiBr_3$ in HBr aq. Red cryst. Probably isostructural with the nonabromide.

Tris-Et_4N salt: Synth. from Et_4NBr + $BiBr_3$ in HBr (aq.). Crimson red cryst. Mp 287° dec.

Tri-Cs salt: see *Tricaesium tri-μ-iodohexaiododibismuthate*(III)(3−), *IC-001537*

Tri-H compd.: see *Trihydrogen tri-μ-iodohexaiododibismuthate*(III)(3−), *IC-001540*

Whealy, R.D. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 479 (*synth*)
Lazarini, F., *Cryst. Struct. Commun.*, 1980, **9**, 815 (*synth, struct*)

$Bi_2Mn_4O_{10}$ IC-001544

Bismuth manganese oxide ($BiMn_2O_5$)

$Bi^{III}_2Mn^{III}_2Mn^{IV}_2O_{10}$

M 797.7

Rhombic struct. with MnO_5 and MnO_6 coordination. Synth. from Bi_2O_3 and Mn_2O_3 or Bi_2O_3 and $MnCO_3$ at 900°. Black metallic cryst.

Bertaut, E.F., *Acta Crystallogr., Sect. A*, 1968, **24**, 217 (*magnetism*)
Niizeki, N. *et al*, *Z. Kristallogr.*, 1968, **127**, 173 (*synth, cryst struct*)
Goshen, S. *et al*, *J. Appl. Phys.*, 1969, **40**, 1590 (*magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1975, C3, 138 (*rev, bibl*)

$Bi_2Mo_3O_{12}$ IC-001545

Bismuth molybdenum oxide ($Bi_2Mo_3O_{12}$)

Bismuth molybdate ($Bi_2(MoO_4)_3$)

[13595-85-2]

$Bi_2(MoO_4)_3$

M 897.7

Phase in the Bi_2O_3-MoO_3 system. Catalyst for oxidation and ammoxidation of alkenes. Microcryst. Mp 660°.

Van den Elzen, A.F. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 2433 (*cryst struct*)
Chen, T. *et al*, *J. Solid State Chem.*, 1975, **13**, 288 (*synth*)
Get'man, E.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 559 (*synth, phase trans*)
Grasselli, R.K., *Appl. Catal.*, 1985, **15**, 127 (*use, rev*)

Theobald, F. *et al*, *Mater. Res. Bull.*, 1985, **20**, 653 (*cryst struct, catalytic activity*)
Antonio, M.R. *et al*, *J. Phys. Chem.*, 1988, **92**, 2939 (*synth, struct*)

Bi_2O_2S IC-001546

Bismuth oxide sulfide (Bi_2O_2S), 11CI

Dibismuth dioxide sulfide

[90014-63-4]

Bi_2O_2S

M 482.0

Bi is coordinated by four O and four S atoms forming square antiprism. The Bi—O bonds form OBi_4 tetrahedra with shared edges forming Bi/O layers. The S atoms link the layers into a three-dimensional network. Bi—O 224.2-239.0, Bi—S 304.0-341.4 pm. Hydrothermal synth., from Bi_2O_3 and Bi_2S_3 in $HO^\ominus$ aq. at 400°/pressure.

Koyama, E. *et al*, *Acta Crystallogr., Sect. B*, 1984, **40**, 105 (*synth, cryst struct*)

Bi_2O_2Se IC-001547

Bismuth oxide selenide (Bi_2O_2Se), 9CI

Dibismuth dioxide selenide

[50811-06-8]

Bi_2O_2Se

M 528.9

Interatomic distances: Bi—O 232, Bi—S 328 pm. Synth. from Bi + Bi_2O_3 + Se in evacuated quartz tube at 800-850°.

Boller, H., *Monatsh. Chem.*, 1973, **104**, 916 (*synth, cryst struct*)

Bi_2O_3 IC-001548

Bismuth oxide (Bi_2O_3), 9CI, 8CI

Bismuth trioxide. Bismuthous oxide. Dibismuth trioxide. Bismuth sesquioxide. Yellow bismuth oxide

[1304-76-3]

M 465.9

Four solid phases recognised with variable polymorphic transitions during cooling. Prepd. by oxidation of Bi by O_2 at 750-800° or by thermal dec. of μ-[Carbonato(2−)-*O*:*O*']dioxodibismuth], IC-002285, Bismuth(*III*) sulfate ($Bi_2(SO_4)_3$), IC-001556, or Bismuth(*III*) nitrate, IC-001516. Occurs in nature as the mineral Bismite. Catalyst for oxidations (and dehydrogenations). Constituent of electrical ceramics, glasses and semiconductors. Formerly employed as a pigment. Yellowish powder, non acidic. Sol. acids; prac. insol. H_2O.

α-form

Monoclinic. Struct. consists of layers of Bi atoms separated by sheets of O atoms. B—O_{av} 235 pm. Synth. from β-form at 650-500° or from Bismuth(*III*) sulfate ($Bi_2(SO_4)_3$), IC-001556 at 950°. Columnar and acicular yellow cryst. At 720-740°, converts into δ-form.

β-form

Tetragonal. Metastable at low temp. Struct. related to fluorite with Bi—O 209.6-246.3 pm, and BiOBi 110.1°, 133.6°. Obt. by cooling δ-form at 650°, or by quenching thin liq. layers. At 650-500°, converts into α-form.

γ-form

Bcc struct. Synth. by cooling δ-form at 640°; struct. may persist at r.t.

δ-form

Disordered fluorite-type struct. Bi—O 231.7 (3×), 309.8 (1×) pm with randomly distributed oxygen vacancies. Synth. from β-form at 660-670° or α-form at 730° or γ-form at 660°. Mp 824°. Converts into β-form at 650° and γ-form at 640°.

[1318-21-4]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 643 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 629 (*rev, bibl*)
Bishay, A.M. *et al*, *Phys. Chem. Glasses*, 1969, **10**, 1 (*glasses, ir, struct*)
Surnina, V.S. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 1695; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 1493 (*synth*)
Morgan, W.E. *et al*, *Inorg. Chem.*, 1973, **12**, 953 (*pe*)
Fomchenkov, L.P. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1974, **10**, 2020; *Inorg. Materials (Engl. Transl.)*, 1974, **10**, 1733 (*synth, props*)
Matsuzaki, R. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 3397 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 601 (*synth*)
Leonhardt, G. *et al*, *Phys. Ser.*, 1977, **16**, 448 (*pe*)
Betsch, R.J. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 505 (*phase diagram, ir, raman*)
Harwig, H.A., *Z. Anorg. Allg. Chem.*, 1978, **444**, 151, 167 (*polymorphs, cryst struct, props*)
Kirk-Othmer Encycl. Chem. Technol., Wiley, N.Y., 1978-1984, **3**, 927 (*rev*)
Harwig, H.A. *et al*, *Thermochim. Acta*, 1979, **28**, 121 (*struct, electrical props*)
Boguslavskii, A.A. *et al*, *Zh. Fiz. Khim.*, 1979, **53**, 33; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1979, **53**, 18 (*ngr*)
Blower, S.K. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 587 (*synth, cryst struct*)
Hill, W.D., *J. Chem. Educ.*, 1989, **66**, 709 (*synth*)
Merck Index, 11th Ed., 1989, No. 1285.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 88 (*haz*)

Bi_2O_5 IC-001549

Bismuth oxide (Bi_2O_5), 9CI, 8CI

Bismuthic oxide. Bismuth(V) *oxide. Dibismuth pentoxide. Bismuth pentoxide (incorr.)*

[35984-07-7]

Bi_2O_5

M 497.9

Not obt. pure, but may exist in several (α, β, γ, δ) phases, all poorly defined. Synth. from bismuth salts + $H_2O_2/HO^\ominus$, Na_2O_2, or peroxydisulfates. Solid, varying in colour from black through light brown to yellow depending on phase. Dec. when heated, and at 350° → Bismuth oxide (Bi_2O_3), IC-001548.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 655 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 644 (*rev, bibl*)
Gattow, G. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **470**, 25 (*synth*)

Bi_2O_5Te IC-001550

Bismuth oxide tellurate (Bi_2O_5Te), 11CI

Bismuth tellurite

[67181-20-8]

Bi_2O_3Te or $Bi_2O_3.TeO_2$

M 625.5

Orthorhombic. Infinite square columns of O atoms along *c*-axis. Synth. from Bi_2O_3-TeO_2 at 700° or from Bi_2TeO_5 at 750°. Insulator. Mp 900°. ΔH −925 kJ mol^{-1}.

Frit, B. *et al*, *Rev. Chim. Minér.*, 1971, **8**, 453 (*struct*)

Mercurio, D. *et al*, *Mater. Chem. Phys.*, 1983, **9**, 467 (*synth, cryst struct*)
Kucha, V.V. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1984, **20**, 314; *Inorg. Materials (Engl. Transl.)*, 1984, **20**, 261 (*synth, cryst struct, ir, uv*)
Gospodinov, G.G. *et al*, *Thermochim. Acta*, 1984, **81**, 349; 1985, **83**, 243 (*synth, props*)
El Farissi, M. *et al*, *Mater. Chem. Phys.*, 1987, **16**, 133 (*synth, cryst struct*)
Mercurio, D. *et al*, *Phys. Status Solidi A*, 1988, **108**, 111 (*struct*)
Földvári, I. *et al*, *J. Crystal Growth*, 1990, **100**, 75 (*synth*)

IC-001551

Bi_2O_6Re

Bismuth rhenium oxide (Bi_2ReO_6)

Bismuth rhenate(VI) (Bi_2ReO_6)

Bi_2ReO_6

M 700.1
Isostruct. with Bi_2MoO_6 mineral. Synth. from Bi_2O_3 and ReO_3 at 450-600°. *p*-type semiconductor.

Kurbanov, T.Kh. *et al*, *Azerb. Khim. Zh.*, 1973, 98; *CA*, **81**, 128677m

IC-001552

Bi_2O_6S

Bismuth oxide sulfate (Bi_2O_6S), 9CI, 8CI

Basic bismuth sulfate

[12010-64-9]

$2Bi_2O_3.Bi_2(SO_4)_3$ or $(BiO)_2SO_4$

M 546.0
Synth. by heating Bismuth(*III*) sulfate ($Bi_2(SO_4)_3$), IC-001556 to 550°; by hydrol. of bismuth sulfate in aq. $OH^{\ominus}$, or from Bi_2O_3 + bismuth sulfate. Mp 1005° (incongr.).

Monohydrate: see *μ-Hydroxyhydroxy-μ-oxo[sulfato(2−)-O] dibismuth*, IC-001539

Aurivillius, B., *Acta Chem. Scand.*, 1964, **18**, 2375 (*cryst struct*)
Margulis, E.V. *et al*, *Zh. Neorg. Khim.*, 1965, **10**, 2304; 1967, **12**, 2036; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 1253; 1967, **12**, 1072 (*synth, cryst struct*)
Aurivillius, B., *Acta Chem. Scand., Ser. A*, 1987, **41**, 415 (*synth*)

IC-001553

$Bi_2O_7Ru_2$

Bismuth ruthenium oxide ($Bi_2Ru_2O_7$), 10CI

Dibismuth diruthenium heptaoxide

[12506-18-2]

$Bi_2Ru_2O_7$

M 732.0
Pyrochlore struct. Prepd. by heating a stoichiometric mixture of Bi_2O_3 and RuO_2 at 1000-1200°. A catalytic material for oxygen electrodes, and useful as a thick-film resistor. Black cryst. (from Bi_2O_3 flux) with metallic conductivity.

Longo, J.M. *et al*, *Mater. Res. Bull.*, 1969, **4**, 191 (*bonding*)
Bouchard, R.J. *et al*, *Mater. Res. Bull.*, 1971, **6**, 669 (*synth, cryst struct*)
Sleight, A.W. *et al*, *NBS Spec. Publ. (U.S.)*, 1972, **364**, 227 (*synth, struct, conductivity*)
Abraham, F. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **280**, 279 (*synth, struct*)
Prosychev, I.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1581 (*synth*)
U.S. Pat., 4 146 458, (1979); *CA*, **90**, 212339 (*use*)
U.S. Pat., 4 176 094, (1979); *CA*, **92**, 31036 (*use, synth*)
Eur. Pat., 13 977, (1980); *CA*, **94**, 75504 (*use*)

$Bi_2O_9S_2$

IC-001554

Bismuth oxide sulfate ($Bi_2O(SO_4)_2$)

Dibismuth monoxy disulfate

[12323-24-9]

$Bi_2O(SO_4)_2$

M 626.0
Monoclinic, contains planar $Bi_4O_2^{8\oplus}$ ions and $[SO_4]^{2\ominus}$ tetrahedra in polymeric struct. Synth. by heating Bismuth(*III*) sulfate ($Bi_2(SO_4)_3$), IC-001556 at ca. 450-500°. Colourless cryst.

α-form
Low temperature-form
Transformed very slowly, to *β*- modification at 532°.

β-form
High temperature-form
Metastable.

Margulis, E.V. *et al*, *Zh. Neorg. Khim.*, 1967, **12**, 2036; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 1072 (*cryst struct, props*)
Jones, W.M., *J. Chem. Phys.*, 1984, **80**, 3408 (*synth, props*)
Aurivillius, B., *Acta Chem. Scand., Ser. A*, 1988, **42**, 95 (*cryst struct*)

$Bi_2O_9Sn_3$

IC-001555

Bismuth tin oxide ($Bi_2Sn_3O_9$), 9CI

Bismuth stannate ($Bi_2(SnO_3)_3$)

[12010-67-2]

$Bi_2(SnO_3)_3$

M 918.0
Used in dielectric ceramics with barium titanate.

▷ EB3130000.

Coffeen, W.M., *J. Am. Ceram. Soc.*, 1953, **36**, 207 (*synth, props*)
Payne, D.A., *Mater. Sci. Res.*, 1986, **20**, 413 (*use, rev*)

$Bi_2O_{12}S_3$

IC-001556

Bismuth(*III*) sulfate ($Bi_2(SO_4)_3$)

$Bi_2(SO_4)_3$

M 706.1
Synth. from Bi dissolved in HNO_3 and evap. with H_2SO_4, with final heating at 380°. Begins to dec. to basic bismuth sulfates at 425°. Easily hydrol. to basic sulfates. Heating with MX (M = Na, Li; X = Cl, Br, I) gives BiX_3.

Lieser, K.H. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **316**, 208 (*props*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 746 (*rev, bibl*)
Margulis, E.V. *et al*, *Zh. Neorg. Khim.*, 1965, **10**, 2304; 1967, **12**, 2036; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 1253; 1967, **12**, 1072 (*synth, props*)
Aurivillius, B., *Acta Chem. Scand., Ser. A*, 1988, **42**, 95.

$Bi_2O_{12}W_3$

IC-001557

Bismuth tungsten oxide ($Bi_2W_3O_{12}$)

Bismuth tungstate ($Bi_2(WO_4)_3$)

[13595-87-4]

$Bi_2(WO_4)_3$

M 1161.5
Phase in the Bi_2O_3-WO_3 system. Green or white cryst. Mp 842°.

Zambonini, F. *et al*, *Gazz. Chim. Ital.*, 1920, **50**, 128 (*synth*)
Smolyaninov, N.P. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 1345 (*formn*)
Sinhamahapatra, P.K. *et al*, *Krist. Tech.*, 1977, **12**, 1205; *CA*, **88**, 1446690q (*cryst struct*)

Bi_2PbS_4

Galenobismuthite **IC-001558**

Bismuth lead sulfide (Bi_2PbS_4)

[12048-53-2]

$PbBi_2S_4$

M 753.4
Mineral, found in gold, bismuth, tungsten and lead-zinc ores as deposits. Mainly USSR and Asia. Grey metallic cryst.

Klyakhin, V.A. *et al*, *Mater. Genet. Eksp. Mineral*, 1972, **7**, 39 (*synth*)
Takeuchi, Y. *et al*, *Proc. Jpn. Acad.*, 1974, **50**, 222 (*cryst struct*)
Chang, L.L.Y. *et al*, *Econ. Geol.*, 1980, **75**, 317 (*synth*)
Friedrich, M., *Bel. Geowiss. Abh., Reihe A*, 1983, **46**, 109.

Bi_2SSe_2

IC-001559

Bismuth selenide sulfide (Bi_2SSe_2), 9CI, 8CI

Dibismuth diselenide sulfide

Bi_2SSe_2

M 607.9
Orthorhombic. Synth. from elements.

Newmann, G. *et al*, *Helv. Phys. Acta*, 1967, **40**, 293 (*synth, cryst struct*)

Bi_2STe_2

IC-001560

Bismuth sulfide telluride (Bi_2STe_2)

Bi_2STe_2

M 705.2
Constituent of the Bi_2S_3-Bi_2Te_3 system. Exists in polymorphic forms which may, however, have different compositions. Synth. from elements at 300-500°. Lead-grey coloured powder. Mp 630° (congr. *γ* phase).

Mineral-form [1304-78-5]
Tetradymite
Suggested composition $Bi_{14}Te_{13}S_8$ with *α*-phase $Bi_{14}Te_{20}S$, *β*-phase $Bi_{14}Te_{15}S_6$, *γ*-phase $Bi_{14}Te_{13}S_8$. Associated with Au ores, and the Bi ores of Hungary. Found in India, Argentina, USSR (several regions), Poland and China.

Glatz, A.C., *Am. Mineral.*, 1967, **52**, 161 (*cryst struct*)
Pauling, L., *Am. Mineral.*, 1975, **60**, 994 (*struct*)
Yusa, K. *et al*, *Sci. Rep. Tohoku Univ., Ser. 3*, 1979, **14**, 121 (*synth, props, cryst struct*)

Bi_2S_3

IC-001561

Bismuth sulfide (Bi_2S_3), 9CI, 8CI

Bismuth(III) *sulfide. Dibismuth trisulfide. Bismuth sesquisulfide*

[1345-07-9]

Bi_2S_3

M 514.1
Each Bi atom has 4 closest neighbours in a nearly planar rectangle and with additional neighbours completing irregular coordinating polyhedra with Bi—S 254-333 pm. Synth. from $Bi(NO_3)_3$ + H_2S; or from Bi + S ; or by dec. of $M(I)_3[Bi(S_2O_3)_3]$ at 200°. Dark brown or black cryst. with metallic lustre. Mp 850°, Mp 685° dec.

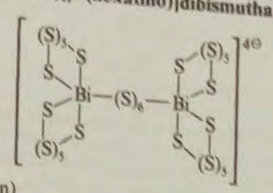
Mineral-form [12233-37-3]
Bismuthinite. Bismuthine. Dismutinite. Bismutholamprite
Occurs with gold deposits and copper ores in parts of the USSR (e.g. Uzbekistan), Europe (Spain, Italy), in the Yukon, and in Brazil.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 730 (*rev, bibl*)
Cambi, L. *et al*, *Chim. Ind. (Milan)*, 1966, **48**, 944 (*synth*)
Kupchik, V. *et al*, *Mineral. Petrogr. Mitt.*, 1970, **14**, 55; *CA*, **73**, 49625 (*cryst struct*)
Popolitov, V.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 2025; *Inorg. Materials (Engl. Transl.)*, 1972, **8**, 1780 (*synth*)
Semin, G.K., *Phys. Status Solidi A*, 1972, **11**, K61 (*ngr*)
Morgan, W.E. *et al*, *Inorg. Chem.*, 1973, **12**, 953 (*pe*)
Kanishcheva, A.S. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1981, **17**, 1972; *Inorg. Materials (Engl. Transl.)*, 1981, **17**, 1466 (*cryst struct*)
Cygański, A. *et al*, *Thermochim. Acta*, 1981, **45**, 65 (*synth*)
Lalia-Kantouri, M. *et al*, *J. Therm. Anal.*, 1984, **29**, 1151 (*synth*)
Wood, S.A. *et al*, *Econ. Geol.*, 1987, **82**, 1864 (*props, synth*)
Steinberg, M. *et al*, *Thermochim. Acta*, 1988, **126**, 199 (*synth, cryst struct*)
Nomura, R. *et al*, *Bull. Chem. Soc. Jpn.*, 1989, **62**, 939 (*synth*)

$Bi_2S_{34}^{4\ominus}$

IC-001562

Tetrakis(heptathio)[μ-(hexathio)]dibismuthate(*III*)(4−)



M 1508.2 (ion)

Tetrakis-Ph_4As salt: [100681-55-8].
Synth. from $BiCl_3$ + polysulfides in the presence of Ph_4AsCl. Dark brown cryst. Triclinic. BiS_7 rings approximate to boat-chair conformations. Highly distorted square pyramidal coordination at Bi. Mean interatomic distances: Bi—S 268.3 (ax), 281.7 pm (eq).

Müller, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1986, **25**, 273 (*synth, ir, raman, cryst struct*)

Bi_2SeTe_2

IC-001563

Bismuth selenide telluride (Bi_2SeTe_2), 9CI, 8CI

Dibismuth selenide ditelluride

[12010-72-9]

Bi_2SeTe_2

M 752.1
Rhombohedral struct. with 5 layer (Se-Bi-Te-Te-Bi) repeating unit. May exist with ordered or disordered Se/Te sub-lattices. Rapid quenching of element melt gives disordered struct., slow cooling gives ordered struct. A phase in Bi_2Te_3/Bi_2Se_3 system. A thermoelectric material.

Mineral-form [79078-60-7]
Kawazulite
The Se analogue of tetradymite. Occurs in a quartz vein in Japan and in a breccia pipe in Canada. Silver to tin white thin foils.

Bland, J.A. *et al*, *Can. J. Phys.*, 1961, **39**, 1040 (*cryst struct*)
Bankina, V.F. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 509 (*formn*)
Gordyakova, G.N. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1191; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 1049 (*thermoelectric props*)
Bhide, V.G. *et al*, *J. Phys. Chem. Solids*, 1971, **32**, 1565 (*struct*)
Gangulee, A. *et al*, *Philos. Mag.*, 8th Ser., 1972, **26**, 337 (*props, struct*)

Miller, R. *et al*, *Can. Mineral.*, 1981, **19**, 341 (*mineral*)
Erofeev, R.R. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1982, **18**, 1802; *Inorg. Materials* (*Engl. Transl.*), 1982, **18**, 1546 (*struct*)
Muragi, B.D. *et al*, *J. Mater. Sci. Lett.*, 1984, **3**, 663 (*cryst struct, formn, ir*)
Dumas, J.F. *et al*, *Thermochim. Acta*, 1987, **122**, 135 (*props*)

Bi_2Se_2Te IC-001564

Bismuth selenide telluride (Bi_2Se_2Te), 11CI
Dibismuth diselenide telluride
[60968-96-9]

Bi_2Se_2Te

M 703.4
Confirmed as component of Bi_2Se_3 – Bi_2Te_3 system.

Muragi, B.D. *et al*, *J. Mater. Sci. Lett.*, 1984, **3**, 663 (*cryst struct, ir, props*)

Bi_2Se_3 IC-001565

Bismuth selenide (Bi_2Se_3), 9CI, 8CI
Bismuth(III) *selenide. Dibismuth triselenide. Bismuth sesquiselenide*
[12068-69-8]

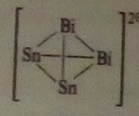
Bi_2Se_3

M 654.8
Has a 15 layer struct. in a rhombohedral subcell. Synth. from Bi + Se at 850° *in vacuo*; or from Bi + Se + Na formate at 312°/100 atm.; or from $Bi(NO_3)_3$ + K_2SeSO_3. Black solid. Mp 710° (695°).

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 762 (*rev, bibl*)
Glazov, V.M. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1966, **2**, 1477; *Inorg. Materials* (*Engl. Transl.*), 1966, **2**, 1262 (*props*)
Krestovnikov, A.N. *et al*, *Zh. Fiz. Khim.*, 1967, **41**, 726; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1967, **41**, 376 (*ms*)
Stasova, M.M. *et al*, *Zh. Strukt. Khim.*, 1967, **8**, 85; *J. Struct. Chem. USSR* (*Engl. Transl.*), 1967, **8**, 69 (*struct*)
Cambi, L. *et al*, *Chim. Ind.* (*Milan*), 1968, **50**, 94 (*synth*)
Boncheva-Mladenova, Z. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1027, 1462; *Inorg. Materials* (*Engl. Transl.*), 1968, **4**, 904, 1279 (*synth, props*)
Klebanov, G.S. *et al*, *Zh. Prikl. Khim.* (*Leningrad*), 1969, **42**, 1715; *J. Appl. Chem. USSR* (*Engl. Transl.*), 1969, **42**, 1617 (*synth*)
Atabaeva, E.Y. *et al*, *Kristallografiya*, 1973, **18**, 173; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1973, **18**, 104 (*cryst struct*)
Kirkinskii, V.A. *et al*, *Zh. Fiz. Khim.*, 1974, **48**, 27; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1974, **48**, 14 (*synth, phase diagram*)
Boechko, V.F. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1975, **11**, 1510; *Inorg. Materials* (*Engl. Transl.*), 1975, **11**, 1288 (*synth, props*)
Richter, W. *et al*, *Phys. Status Solidi B*, 1977, **84**, 619 (*ir, raman, struct*)
Thuler, M.R. *et al*, *Chem. Phys.*, 1982, **71**, 265 (*pe*)
Satow, T. *et al*, *Phys. Status Solidi A*, 1982, **71**, 555 (*ed, struct*)

$Bi_2Sn_2^{2\ominus}$ IC-001566

Dibismuthatedistannate(2 –)



M 655.3 (ion)
Tetrahedral cluster anion.
Bis[(*222-cryptand*)-*K*] *salt, compd. with ethylenediamine*: [82167-47-3].
Synth. from KSn_2 and K_3Bi_2 with cryptand-222 in ethylenediamine. Black plates.

Critchlow, S.C. *et al*, *Inorg. Chem.*, 1982, **21**, 3286 (*synth, cryst struct*)
Birchall, T. *et al*, *Inorg. Chem.*, 1985, **24**, 890 (*mössbauer*)

Bi_2Te_3 IC-001567

Bismuth telluride (Bi_2Te_3), 9CI, 8CI
Dibismuth tritelluride. Bismuth sesquitelluride
[1304-82-1]

Bi_2Te_3

M 800.7
Layer struct. when unit cell in tetradymite hexagonal lattice. Synth. from Bi + Te at 700°, or from Bi_2O_3 + Te + Na formate at *ca.* 300°/100 atm. Semiconductor employed in industrial thermoelectrical technology. Films are ir photosensitive. Grey solid. Mp 586° (573°) (incongr.). Vap. completely dissociated.
▷ EB3110000.

Mineral-form [12068-70-1]
Tellurobismuthite
Widespread in USSR. Also occurs in Sweden, Canada. V. often in gold ores and complex sulfide ores.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Supp. Vol.*, 1964, 788 (*rev, bibl*)
Boncheva-Mladenova, Z. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1966, **2**, 1542; *Inorg. Materials* (*Engl. Transl.*), 1966, **2**, 1324 (*synth, props*)
Gorbov, S.I. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1966, **2**, 1702; *Inorg. Materials* (*Engl. Transl.*), 1966, **2**, 1465 (*props, ms*)
Stasova, M.M. *et al*, *Zh. Strukt. Khim.*, 1967, **8**, 85; *J. Struct. Chem. USSR* (*Engl. Transl.*), 1967, **8**, 69 (*cryst struct*)
Cambi, L. *et al*, *Chim. Ind.* (*Milan*), 1968, **50**, 869 (*synth, cryst struct*)
Atabaeva, E.Y. *et al*, *Fiz. Tverd. Tela* (*Leningrad*), 1968, **10**, 62; *Soviet Physics: Solid State*, 1968, **10**, 43 (*synth, props*)
Boncheva-Mladenova, Z. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 1264; *Inorg. Materials* (*Engl. Transl.*), 1970, **6**, 1109 (*reactions*)
Richter, W. *et al*, *Phys. Status Solidi B*, 1977, **84**, 619 (*ir, raman, struct*)
Vasil'eva, N.D. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1978, **14**, 1430; *Inorg. Materials* (*Engl. Transl.*), 1978, **14**, 1116 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **22**, 900 (*uses*)
Thuler, M.R. *et al*, *Chem. Phys.*, 1982, **71**, 265 (*pe*)
Galetskaya, A.D. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1982, **18**, 1820; *Inorg. Materials* (*Engl. Transl.*), 1982, **18**, 1563 (*synth*)
Satow, T. *et al*, *Phys. Status Solidi A*, 1982, **71**, 555 (*synth, struct*)
Merck Index, 10th Ed., 1983, No. 1288.
Chassé, T. *et al*, *Cryst. Res. Technol.*, 1985, **20**, 1475 (*pe*)
Nadzhip, A.E. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1987, **25**, 1458; *Inorg. Materials* (*Engl. Transl.*), 1987, **25**, 1234 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 524 (*haz*)

Bi_5BrO_4 IC-001568

Bismuth bromide oxide (Bi_5BrO_4), 11CI
Tribismuth bromide tetroxide
[87970-85-2]

Bi_3BrO_4 or $Bi_2O_3.BiOBr$

M 770.8
Orthorhombic. Bi atoms form the apices of flat BiO_3 tetrahedra which are joined to form chains. L.p. is stereochemically active. Bi—Br 330-370. Bi—O 219-286 pm. At least 3 polymorphs reported. Synth. from Bi_2O_3 + BiOBr at 870° in gold capsule; or from Bi_2O_3 + $BiBr_3$ in Pt vessel at 700°. Yellowish powder.

Nurgaliev, B.Z. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 2207; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1252 (*synth, cryst struct*)
Aurivillius, B., *Chem. Scr.*, 1984, **24**, 125 (*synth, cryst struct*)

Bi_3ClO_4 IC-001569

Bismuth chloride oxide (Bi_3ClO_4), 11CI
Tribismuth chloride tetroxide
[87970-86-3]

Bi_3ClO_4

M 726.3
Monoclinic, body-centred struct. Synth. from Bi_2O_3 + $BiCl_3$ in Pt at 700° or from Bi_2O_3 in $Cl^\ominus$ soln. at pH > 6. White or pale yellow clusters of platelets.

Nurgaliev, B.Z. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 2207; 1985, **30**, 1665; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1252; 1985, **30**, 948 (*synth, cryst struct*)

Bi_3O_8Re IC-001570

Bismuth rhenium(*VII*) oxide (Bi_3ReO_8), 11CI
Bismuth oxide rhenate(VII) ($Bi_3O_3(ReO_4)$)
[73079-50-2]

Bi_3ReO_8

M 941.1
Has a cubic struct. related to fluorite, with ReO_4 tetrahedra rotated to accommodate Bi lone pairs. Re—O 172.8 to 175.3 pm. Synth. from Re_2O_7 and Bi_2O_3 at ~400°. Colourless cryst.; bulk material pale cream-coloured. Mp 1473°. Ir ν_{ReO} 900 cm^{-1}.

Cheetham, A.K. *et al*, *Mater. Res. Bull.*, 1981, **16**, 7 (*synth, ir, struct*)
Cheetham, A.K. *et al*, *Acta Crystallogr., Sect. B*, 1985, **41**, 225 (*cryst struct*)

$Bi_3O_{11}Ru_3$ IC-001571

Bismuth ruthenium oxide ($Bi_3Ru_3O_{11}$), 10CI
Tribismuth triruthenium undecaoxide
[58833-98-0]

$Bi_3Ru_3O_{11}$

M 1106.1
Struct. similar to Lanthanum ruthenium oxide ($La_4Ru_6O_{19}$), IC-020577, Ru—Ru 260 pm indicating strong localised Ru—Ru bonding. Prep. by heating Bi_2O_3 with RuO_2 (mol ratio 1:2) at <975° in air. Cubic cryst. Dec. to $Bi_2Ru_2O_7$ at temps. >975°.

Abraham, F. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **278**, 421 (*synth, cryst struct*)
Abraham, F. *et al*, *Bull. Soc. Fr. Minéral. Cristallogr.*, 1975, **98**, 25 (*synth, cryst struct*)

$Bi_4Br_2O_5$ IC-001572

Bismuth bromide oxide ($Bi_4Br_2O_5$), 11CI
Tetrabismuth dibromide pentoxide
[87970-87-4]

$Bi_4Br_2O_5$

M 1075.7
Monoclinic. Non-centrosymmetric struct. to 300°. Synth. from Bi_2O_3 + $BiBr_3$ at 800° in Pt. Solid.

Nurgaliev, B.Z. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 2207; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1252 (*synth, cryst struct*)

Bi_4ClNbO_8 IC-001573

Bismuth niobium chloride oxide (Bi_4NbClO_8), 11CI
Tetrabismuth chlorooctaoxoniobium(V)
[91261-86-8]

$(Bi_2O_2)_4(NbO_4)_2Cl_2$

M 1092.2
The unit cell contains four Bi_2O_2, two NbO_4 and two Cl layers. The Nb layers are formed by distorted octahedra sharing edges and canted relative to one another. Synth. by heating Bi_2O_3, BiOCl and Nb_2O_5 to 950° in a Pt tube. The bromide and the corresponding Ta compd. are also known.

Aurivillius, B., *Chem. Scr.*, 1984, **23**, 143 (*cryst struct*)
Ackerman, J.F., *J. Solid State Chem.*, 1986, **62**, 92 (*synth, cryst struct*)

$Bi_4Cl_2O_5$ IC-001574

Bismuth chloride oxide ($Bi_4Cl_2O_5$), 9CI
Tetrabismuth dichloride pentoxide
[60674-93-3]

$Bi_4Cl_2O_5$

M 986.8
Orthorhombic. Bi atoms coordinated by (1) 4 oxygens in sq. pyramid with l.p. at apex (Bi—O 236-249 pm) or (2) 5 oxygens in octahedron with l.p. at corner (Bi—O 213-246 pm). The polyhedra are linked by shared edges and corners forming infinite layers. $Cl^\ominus$ ions form parallel trigonal prisms between Bi—O layers. Synth. from Bi_2O_3 + BiOCl in sealed Au capsule at *ca.* 850°. Colourless needle-like cryst.

Hopfgarten, F., *Acta Crystallogr., Sect. B*, 1976, **32**, 2570; 1977, **33**, 952 (*synth, cryst struct*)
Kodama, H. *et al*, *J. Solid State Chem.*, 1988, **75**, 279 (*synth, cryst struct*)

$Bi_4Cl_2S_5$ IC-001575

Bismuth chloride sulfide ($Bi_4Cl_2S_5$), 10CI
Tetrabismuth dichloride pentasulfide
[61393-72-4]

$Bi_4Cl_2S_5$

M 1067.1
Rhombohedral. Struct. has statistical occupancy of sites by S and Cl. Unusual coordination polyhedra around Bi. One Bi has 9 S or Cl neighbours at 288, 290, 344 pm. The remaining 3 Bi atoms are irregularly surrounded each by 8 S or Cl atoms at 262-366 pm. Synth. from BiSCl heated at 350° under N_2, or from BiSCl + Bi_2S_3 heated at 340°. Dark grey solid. $\Delta H^\circ_{f,298}$ –593 kJ mol^{-1}.

Krämer, V., *Z. Naturforsch., B*, 1976, **31**, 1542 (*synth, cryst struct*)
Krämer, V., *Acta Crystallogr., Sect. B*, 1979, **35**, 139 (*cryst struct*)
Vorob'eva, T.A. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 767; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 428 (*synth, thermodyn, phase diagram*)

Bi_4O_5 IC-001576

Bismuth oxide (Bi_4O_5), 9CI, 8CI
Tetrabismuth pentoxide
[11078-75-4]

Bi_4O_5

M 915.9

May be identical to the β-phase of Bismuth oxide (Bi_2O_3), IC-001548. Tetragonal cell in which each Bi atom is surrounded by 6 oxygens (trigonal prism) and each O by 4 bismuth atoms (tetrahedron) with Bi—O 214-218 pm and minimum Bi—Bi 375 pm; up to 25% deficiency in oxygen sub lattice. Synth. from Bi + O_2 at 200-250°.

Zav'yalova, A.A. *et al, Kristallografiya*, 1971, **16**, 516; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1971, **16**, 437 (*struct, synth*)
Zav'yalova, A.A. *et al, Zh. Strukt. Khim.*, 1972, **13**, 869; *J. Struct. Chem. USSR (Engl. Transl.)*, 1972, **13**, 811 (*struct*)
Pinskei, Z.G. *et al, Thin Solid Films*, 1976, **32**, 287 (*synth, struct*)

IC-001577

Bi_4Se_3

Bismuth selenide (Bi_4Se_3)

Tetrabismuth triselenide

[12233-59-9]

Bi_4Se_3

M 1072.8

Rhombohedral layer struct. with 21 layer periodicity: SeBiSeBiSe packs between which are distributed doubly covalently bonded Bi layers. Synth. from the elements. V. soft, readily deformable lamellar platelets.

Stasova, M.M. *et al, Zh. Strukt. Khim.*, 1967, **8**, 85, 655; *J. Struct. Chem. USSR (Engl. Transl.)*, 1967, **8**, 69, 584 (*cryst struct*)
Stasova, M.M., *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 28; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 21 (*struct*)

IC-001578

Bi_4Te_3

Bismuth telluride (Bi_4Te_3), 10CI

Tetrabismuth tritelluride

[69431-11-4]

Bi_4Te_3

M 1218.7

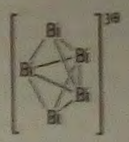
Rhombohedral. Structurally characterised by combination of 5 layers (TeBiTeBiTe). (Te—Bi, 311.5, 332.7, 340.1 pm) with two layers BiBi (Bi—Bi 309.8 pm). Synth. from the elements at 800°.

Yamana, K. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 147 (*synth, cryst struct*)

IC-001579

$Bi_5^{3\oplus}$

Pentabismuth(3+)



M 1044.9 (ion)

Tris(tetrachloroaluminate): [12301-55-2].
$Al_3Bi_5Cl_{18}$ M 1551.2
Synth. from Bi, $BiCl_3$ and $AlCl_3$ at 250-270° in $KAlCl_4$ or $NaAlCl_4$. Red-brown air and moisture sensitive cryst. (molten $NaAlCl_4$). Mp 326°.

Tris(hexafluoroarsenate): [68002-15-3].
$As_3Bi_5F_{18}$ M 1611.6
Synth. from AsF_5 + Bi in $SO_2(l)$. Bright yellow solid. Slowly oxidised in conc. H_2SO_4.

Corbett, J.D. *et al, Inorg. Chem.*, 1968, **7**, 198 (*synth, props*)
Corbett, J.D. *et al, Prog. Inorg. Chem.*, 1976, **21**, 129 (*rev*)
Burns, R.C. *et al, Inorg. Chem.*, 1978, **17**, 3596 (*synth, str, ir, raman*)

IC-001580

Bi_5BrO_7

Bismuth bromide oxide (Bi_5BrO_7), 11CI

[89190-54-5]

Bi_5BrO_7 or $BiOBr.2Bi_2O_3$

M 1236.8

Synth. from Bi_2O_3 + $BiBr_3$ → polycryst. at 600°, BiOBr + $OH^{\ominus}$ → single cryst.

Ketterer, J. *et al, Z. Naturforsch., B*, 1984, **39**, 105 (*synth, cryst struct*)

IC-001581

Bi_5IO_7

Bismuth iodide oxide (Bi_5IO_7), 9CI

Pentabismuth iodide heptoxide

[53908-32-0]

Bi_5IO_7 or $BiIO.2Bi_2O_3$

M 1283.8

Two polymorphs recognised. Synth. from BiIO + 5*M* KOH aq. or by heating BiIO at 370° in O_2. Candidate material for immobilisation of radioactive iodine. Yellow solid. Mp 855° (incongr.). At 490° → Bi_2O_3 in O_2.

α-form

Orthorhombic. From BiIO + excess KOH aq., or α-Bi_2O_3 + HI aq.

β-form

Monoclinic. Struct. contains 5 cryst. independent Bi atoms with $[Bi_{10}O_{14}]_n^{2n\oplus}$ columns connected by double rows of iodine atoms. Produced in small amount together with α-form. Colourless solid. In sealed system stable to *ca.* 800° when dec. → Bi_2O_3 + BiI_3.

Gmelin Handbook Inorg. Chem., Syst. No. 19, *Suppl. Vol.*, 1964, 722 (*rev, bibl*)
Klimakov, A.M. *et al, Zh. Neorg. Khim.*, 1974, **19**, 2553; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 1394 (*phase diagram*)
Rulmont, A., *Rev. Chim. Minér.*, 1977, **14**, 277 (*synth, cryst struct*)
Ketterer, J. *et al, Z. Naturforsch., B*, 1984, **39**, 105 (*synth, cryst struct*)
Ketterer, J. *et al, Z. Kristallogr.*, 1985, **172**, 63 (*synth, cryst struct*)
Taylor, P. *et al, Can. J. Chem.*, 1986, **64**, 290; 1988, **66**, 2664 (*synth*)

IC-001582

$Bi_5O_{10}P$

Bismuth oxide phosphate ($Bi_5O_6(PO_4)$), 9CI

[51311-06-9]

$Bi_5O_6(PO_4)$

M 1235.8

Synth. from Bi_2O_3 + $NH_4.H_2PO_4$ at 300°, then at 700-800° in Pt vessel. Pale yellow cryst. Mp 965°.

Brixner, L.H. *et al, Mater. Res. Bull.*, 1973, **8**, 1311 (*synth, cryst struct*)

IC-001583

Bi_6Cl_7

Bismuth chloride (Bi_6Cl_7), 8CI

Hexabismuth heptachloride. Bismuth monochloride

$(Bi_6^{5\oplus})_2(BiCl_5^{2\ominus})_4(Bi_2Cl_8^{2\ominus})$ (tetramer)

M 1502.0

Referred to in earlier lit. as BiCl. Now known to be a 'tetramer'. Contains the Nonabismuth(5+), IC-001587 cation.

Tetramer: Bismuth chloride ($Bi_{24}Cl_{28}$).
Bis(nonabismuth(5+)) octachlorodibismuthate(2−) tetrakis(pentachlorobismuthate(2−))
$Bi_{24}Cl_{28}$ M 6008.2
Synth. from Bi + $BiCl_3$ at 325°. Shiny black prisms with flattened hexagonal cross-sections; dec. slowly in air. Diamagnetic. Stable *in vacuo* to 200°. Cation is tripyramidal trigonal prism with Bi atoms projecting from each face: geometry distorted by unsymm. environment of nearby anions. Anions are tetragonal pyramidal $BiCl_5^{2\ominus}$, and $Bi_2Cl_8^{2\ominus}$ formed by two $BiCl_5^{2\ominus}$ groups sharing two Cl's, Bi—Cl 261-278, Bi—Bi 308, 329 pm.

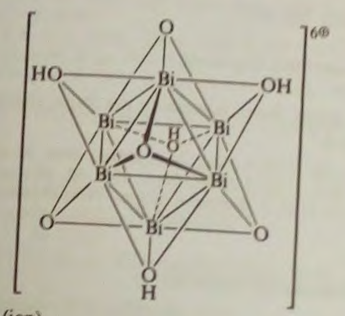
Hershaft, A. *et al, Inorg. Chem.*, 1963, **2**, 979 (*synth, cryst struct*)
Corbett, J.D. *et al, Inorg. Chem.*, 1964, **3**, 1408 (*struct*)

$Bi_6H_4O_8^{6\oplus}$

IC-001584

Tetra-μ$_3$-hydroxytetra-μ$_3$-oxohexabismuth(6+), 11CI

[85507-34-2]



M 1385.9 (ion)

Hexanitrate, tetrahydrate: [69756-07-6].
Synth. by hydrol. of Bismuth(*III*) nitrate, IC-001516 at pH < 1. Earlier formulated as $BiONO_3.H_2O$, or as $Bi_2O_3.N_2O_5.2H_2O$, but appears to be a true hydrate. Thermal dec. starts at ~40°. Loses $2H_2O$ at up to 110°, and two more H_2O at up to 120°. Dehydration complete at 150°.

Hexaperchlorate, heptahydrate: Formed during pptn. of $Bi(OH)_3$ from $Bi(ClO_4)_3$ soln.; and during diln. of $Bi(ClO_4)_3$ soln.; also from Bi_2O_3 + 3M $HClO_4$ aq. Deliquescent, colourless cryst. Orthorhombic. Discrete ion complexes. Formerly represented as $[Bi(OH)_6^{6\oplus}][ClO_4^{\ominus}]_6$.

[12441-70-2, 18866-22-3]

Levy, H.A. *et al, J. Chem. Phys.*, 1959, **31**, 1458 (*perchlorate, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 19, 1964, 647 (*rev, bibl*)
Maroni, V.A. *et al, J. Am. Chem. Soc.*, 1966, **88**, 1410 (*ir, raman*)
Maroni, V.A. *et al, Inorg. Chem.*, 1968, **7**, 183 (*ir, raman*)
Quicksall, C.O. *et al, Inorg. Chem.*, 1970, **9**, 1045 (*raman*)
Frit, V. *et al, Ber. Bunsenges. Phys. Chem.*, 1973, **77**, 243 (*synth*)
Lazarini, F. *et al, Cryst. Struct. Commun.*, 1979, **8**, 69 (*nitrate, cryst struct*)
Burkov, K.A. *et al, Koord. Khim.*, 1979, **5**, 1328 (*synth, raman*)
Lazarini, F. *et al, Thermochim. Acta*, 1981, **46**, 53 (*props*)
Sundvall, B., *Inorg. Chem.*, 1983, **22**, 1906 (*perchlorate, cryst struct, ref*)
Gentile, I. *et al, Inorg. Chem.*, 1985, **24**, 2405 (*pmr, struct*)

IC-001585

$Bi_6H_6NO_{12}^{5\oplus}$

Aquatetra-μ$_3$-hydroxy(nitrato-*O*)-tetra-μ$_3$-oxohexabismuth(5+), 10CI

[69716-44-5]

$[Bi_6(OH_2)(NO_3)O_4(OH)_4]^{5\oplus}$

M 1465.9 (ion)

Pentanitrate:
$Bi_6H_6N_6O_{27}$ M 1615.9
Synth. by hydrol. below pH 2.4 of $Bi(NO_3)_3$. Also formulated as $[Bi_6O_4](NO_3)_6.3H_2O$ or as $2BiO.NO_3.H_2O$ or $Bi_2O_3.N_2O_5.H_2O$ Monoclinic. The Bi atoms are at the corners of an octahedron with O's and and OH groups above the centre of the octahedron faces. Each O of each OH has 3 Bi neighbouring atoms arranged pyramidally at long distances. The remaining O's are linked to 3 nearly coplanar Bi's at shorter distances. Bi—O 210-263 pm. $NO_3^{\ominus}$ and H_2O bound to neighbouring Bi atoms.

[10361-46-3, 70341-25-2]

Gattow, G. *et al, Z. Anorg. Allg. Chem.*, 1963, **324**, 31; 1965, **335**, 61 (*synth*)
Sundvall, B., *Acta Chem. Scand., Ser. A*, 1979, **33**, 219 (*cryst struct*)
Lazarini, F. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 448 (*synth, cryst struct*)

IC-001586

$Bi_6O_{15}Te_2$

Bismuth oxide tellurate ($Bi_6O_9(TeO_6)_2$)

[53322-38-6]

$Bi_6O_9(TeO_6)_2$ or $3Bi_2O_3.2TeO_3$

M 1749.0

Orthorhombic. Synth. from Bi_2O_3 + TeO_2 + O_2 at 650°. Solid. Stable to 850°, although sl. struct. change at 740°. At high temp. → O_2 + basic Bi tellurite.

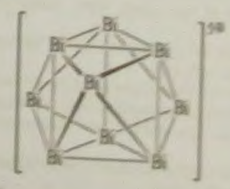
Frit, B. *et al, Bull. Soc. Chim. Fr.*, (Part 1), 1974, 402 (*synth, cryst struct*)
Gospodinov, G.G. *et al, Thermochim. Acta*, 1985, **83**, 243; **91**, 364 (*synth, cryst struct, props*)

IC-001587

$Bi_9^{5\oplus}$

Nonabismuth(5+)

[39448-36-7]



M 1880.8 (ion)

One of a series of bismuth polycations, originally discovered as a component of Bismuth chloride (Bi_6Cl_7), IC-001583.

Bi(1+), tris-hexachlorohafnate(2−): [12591-16-1].
Bismuth(1+) nonabismuth(5+) tris(hexachlorohafnate(2−))
$Bi_{28}Cl_{18}Hf_3$ M 3263.4
Synth. from Hf + $2BiCl_3$ + $3HfCl_4$ melt. Needles. Mp 507° (incongr.). This sp. contains first example of Bi(1+) in solid state.

$(BiCl_5)_4^{2\ominus}$ $(Bi_2Cl_8)^{2\ominus}$ *salt:* see *Bismuth chloride* (Bi_6Cl_7), *IC-001583*
Friedman, R.M. *et al*, *Inorg. Chem.*, 1973, **12**, 1134 (*synth, ir, cryst struct, magnetism*)

IC-001588

$Bi_{12}Cl_2O_{17}$

Bismuth chloride oxide ($Bi_{12}Cl_2O_{17}$), 11Cl

[87970-89-6]

$Bi_{12}Cl_2O_{17}$

M 2850.6
Synth. from Bi_2O_3 + $BiCl_3.H_2O$ heated in quartz or Pt. Aggregates of fine yellow platelets. With aq. alkali gives Bi_2O_3.
Nurgaliev, B.Z. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 2207; 1985, **30**, 1665; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1252; 1985, **30**, 948 (*synth, cryst struct*)
Taylor, P. *et al*, *Can. J. Chem.*, 1987, **65**, 2824 (*formn, props*)
Koduma, H. *et al*, *J. Solid State Chem.*, 1988, **75**, 279 (*synth*)

IC-001589

Bk

Berkelium

[7440-40-6]

Bk

M 249.0
Atomic No. 97. Ground state electron config. $[Rn]5f^97s^2$ or $[Rn]5f^86d^17s^2$. 11 Isotopes are known. Only ^{249}Bk available for chem. study. Produced by Thompson, Ghiorso and Seaborg in 1949 at Berkeley, Calif. α-Form (double hcp) and r.t. metastable fcc form exist, with transformation at 930°. Obt. by neutron bombardment of Pu, Am, Cm. Metal obt. by redn. of BkF_3, BkF_4 with Li or BkO_2 with Th or La. No practical applications. Silvery metal. Possibly forms oxide film. Attacked by steam. Reacts rapidly with dil. HCl or other mineral acids. Combines directly with H_2, N_2, P, As, Sb, Se, etc. Mp 986° (meas.), Mp *ca.* 1050° (est.). Bp *ca.* 2623° (est.).

▷ Radioactive.

Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 859 (*history*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **5**, 5 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **1**, 456; **19**, 639, 682 (*rev, bibl*)
Peterson, J.R. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1984, **28**, 29 (*rev*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 1450 (*rev*)
Hobart, D.E. *et al*, *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, 989 (*rev*)
Spirlet, J.R. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1987, **31**, 1 (*rev, bibl*)
Seaborg, G.T. *et al*, *The Elements Beyond Uranium*, Wiley-Interscience, 1990 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 28.

$BkBr_3$

IC-001590

Berkelium(*III*) bromide ($BkBr_3$)

Berkelium tribromide

[22787-71-9]

$BkBr_3$

M 488.7
Exists in three cryst. modifications. Orthorhombic, with the $PuBr_3$ struct., monoclinic,with $CrCl_3$ struct., and rhombohedral with the $BiCl_3$ struct. Light green or yellow-green solid. Also formed on α-decay of $EsBr_3$.

[24297-28-7]

Cohen, D. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 257 (*synth, struct*)
Burns, J.H. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 743 (*synth, cryst struct*)
Peterson, J.R. *et al*, *Rev. Chim. Minér.*, 1977, **14**, 172.
Young, J.P. *et al*, *Inorg. Chem.*, 1981, **20**, 3979 (*synth, uv-vis*)

$BkCl_3$

IC-001591

Berkelium(*III*) chloride ($BkCl_3$)

Berkelium trichloride

[13536-46-4]

$BkCl_3$

M 355.4
Green solid. Mp 603°.

α-form

Possesses the UCl_3 struct.

β-form

High temps. form, possessing the $PuBr_3$ struct.

[20063-16-5]

Peterson, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 823 (*synth*)
Carnall, W.T. *et al*, *J. Chem. Phys.*, 1973, **58**, 3614 (*uv-vis*)
Young, J.P. *et al*, *J. Radioanal. Chem.*, 1978, **43**, 479 (*synth*)

$BkCl_6^{3\ominus}$

IC-001592

Hexachloroberkelate(*III*)(3−)

$BkCl_6^{3\ominus}$

M 461.7 (ion)
Na, di-Cs salt: [12431-46-8].
$BkCl_6Cs_2Na$ M 750.5
White solid. 6-Coord. Bk, having the Cryolite struct.
Morss, L.R. *et al*, *Inorg. Chem.*, 1969, **8**, 1433 (*synth, struct*)

$BkCl_6^{2\ominus}$

IC-001593

Hexachloroberkelate(*IV*)(2−)

[34390-41-5]

$[BkCl_6]^{2\ominus}$ (O_h)

M 461.7 (ion)
Di-Cs salt: [25395-77-1].
$BkCl_6Cs_2$ M 727.6
Orange cryst. Isostructural with Rb_2MnF_6.

[12431-45-7]

Morss, L.R. *et al*, *Inorg. Chem.*, 1969, **8**, 1433 (*synth, struct*)
Jenkins, H.D.B. *et al*, *Prog. Solid State Chem.*, 1979, **12**, 125.

BkF_3

IC-001594

Berkelium(*III*) fluoride (BkF_3)

Berkelium trifluoride

[20716-88-5]

BkF_3

M 306.0
Yellow-green solid.

Orthorhombic-form

R.t. form, isostructural with YF_3, having 8-coord. Bk.

Trigonal-form

High temp. form, with the LaF_3 struct.

[20063-17-6]

Peterson, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 1775 (*synth, struct*)
Ensor, D.D. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 1001, 2425 (*synth, uv-vis*)

BkF_4

IC-001595

Berkelium(*IV*) fluoride (BkF_4)

Berkelium tetrafluoride

[22422-77-1]

BkF_4

M 325.0
Possesses the UF_4 struct. Synth. from BkO_2 + F_2 (400°). Pale yellow-green solid.

[87345-81-1]

Asprey, L.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 537; 1973, **9**, 1121 (*synth, struct*)
Keenan, T.K. *et al*, *Inorg. Chem.*, 1969, **8**, 235 (*struct*)
Haug, H.O. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 847 (*struct*)
Ensor, D.D. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 1001 (*synth, uv-vis*)
Nave, S.E. *et al*, *Phys. Rev. B*, 1983, **28**, 2317 (*magnetism*)

[BkH]

IC-001596

Berkelium hydrides

Berkelium hydride (BkH$_2$) [98790-54-6]
BkH_2 M 251.0
Has fluorite struct. Non-stoichiometric: BkH_{2+x}. Grey solid.

Berkelium hydride (BkH$_3$) [98790-55-7]
BkH M 250.0
Has LaF_3 struct. Non-stoichiometric: BkH_{3-x}.

[98790-55-7]

Fahey, J.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 101 (*BkH_3*)
Gibson, J.K. *et al*, *J. Less-Common Met.*, 1985, **109**, 251 (*synth, BkH_2, BkH_3*)

BkI_3

IC-001597

Berkelium(*III*) iodide (BkI_3)

Berkelium triiodide

[23171-53-1]

BkI_3

M 629.7
Possesses the BiI_3 struct. Formed in α-decay of EsI_3. Yellow solid. Bp 650° (*in vacuo*).

[89759-76-2]

Cohen, D. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 257 (*synth, struct*)
Young, J.P. *et al*, *Inorg. Chem.*, 1981, **20**, 3979 (*synth, uv-vis*)

BkN

IC-001598

Berkelium nitride (BkN)

[56509-31-0]

BkN

M 263.0
NaCl struct. Cryst. solid.

[51366-65-5, 70420-42-7]
Stevenson, J.N. *et al*, *J. Less-Common Met.*, 1979, **66**, 201 (*synth, struct*)
Damien, D. *et al*, *J. Phys. Colloq.*, 1979, **4**, 95 (*synth, struct*)
Damien, D. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **42**, 995.

BkO_2

IC-001599

Berkelium(*IV*) oxide (BkO_2)

Berkelium dioxide

[12010-84-3]

BkO_2

M 281.0
Has fluorite struct. First Bk compd. to be identified. Brown solid.

Peterson, J.R. *et al*, *Inorg. Nucl. Chem. Lett.*, 1967, **3**, 327 (*synth, struct*)
Baybarz, R.D., *J. Inorg. Nucl. Chem.*, 1973, **35**, 4149; 1968, **30**, 1769 (*synth, struct*)
Fahey, J.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1974, **10**, 459 (*synth*)
Sudakov, L.V. *et al*, *Sov. Radiochem.* (*Engl. Transl.*), 1977, **19**, 394 (*synth*)

Bk_2O_3

IC-001600

Berkelium(*III*) oxide (Bk_2O_3)

Diberkelium trioxide. Berkelium sesquioxide

[12310-58-6]

Bk_2O_3

M 546.1
3 forms known in solid state. Mp 1920°.

A-form

High-temp-form
Hexagonal. Stable above 2025°.

B-form

Medium-temp-form
Monoclinic. Stable between ~1473-2025°.

C-form

Low-temp-form
Cubic. Stable at r.t. and up to ~1473°.

Peterson, J.R. *et al*, *Inorg. Nucl. Chem. Lett.*, 1967, **3**, 327 (*synth*)
Baybarz, R.D., *J. Inorg. Nucl. Chem.*, 1968, **30**, 1769; 1973, **35**, 4149 (*synth, struct*)
Fournier, J.M., *J. Phys. Chem. Solids*, 1976, **37**, 235.

Br

IC-001601

Bromine, 11Cl

Dibromine

[7726-95-6]

Br_2

M 79.9
Atomic No. 35. Ground state electron config. [Ar] $3d^{10}4s^24p^5$. Isol. in 1826 by A.J. Balard and C. Löwig. Abundance: 2.5 ppm (earth's crust) and 65 ppm (sea water). Br—Br: 228 pm, 227 pm (solid). Also occurs naturally in several marine species. There are 19 isotopes of which ^{79}Br and ^{81}Br are natural and are of importance in nmr spectroscopy. Obt. as bromide from natural brines from wells in USA. Oxidation by air gives the element. Synth. from metallic bromides by reaction with oxidants (e.g. $K_2Cr_2O_7/H_2SO_4$). Liberated from brines on chlorination. Used in making lead scavenging agents, fumigants, flameproofing agents, water purifn. prods., and many fine chemicals with wide applications. Dark brownish-red liq., with a strong disagreeable pungent odour, forming rhombic cryst. Strong oxidant. Sol. H_2O (3% at r.t.) increased in

presence of bromide salts. Misc. most org. solvs. (although it may react). d^{20} 3.12 (l). Mp −7.3°. Bp 59.5°. Forms adducts with many org. compds. (e.g. ethers such as dioxan, and aromatic hydrocarbons) and also hydrates. Dissociates at > 600°. Bond energy 193 kJ mol^{-1}.

▷ Causes painful burns on skin contact; irritates eyes and throat. EF9100000.

Octahydrate: Light red cryst. Cubic. May be stored at r.t. at < 6.2°.

[10097-32-2, 11094-39-6, 12595-73-2, 14336-94-8, 14380-59-7]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1922, **2**, 15; *Suppl. Vol.* 1, 1956, 689 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 7, 1931; *Suppl. Vol.*, 1985, **A** (*rev, bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1972, **3**, 34; **4**, 46; **5**, 55; **6**, 70 (*uses*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1107 (*rev, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 290 (*synth*)
Lindman, B. *et al, NMR and the Periodic Table*, (R.K. Harris *et al*, Ed.), Academic Press, London, 1978, 421 (*nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 226; **24**, 391 (*rev, bibl*)
Soulard, M. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 2300 (*uv, reaction*)
Johanssen, P.-G. *et al, J. Phys. C*, 1983, **16**, 1961 (*solid, raman*)
Powell, B.M. *et al, Mol. Phys.*, 1984, **53**, 929 (*cryst struct*)
Greenwood, N.N. *et al, Chemistry of the Elements*, Pergamon, Oxford, 1986, 920 (*rev*)
Emsley, J., *The Elements*, 2nd Ed., Clarendon Press, Oxford, 1991, 36.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 555 (*tox*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 97 (*haz*)

BrCa$_5$O$_{12}$P$_3$ IC-001602

Calcium bromide phosphate ($Ca_5Br(PO_4)_3$), 9CI

Calcium bromapatite

[12514-27-1]

$Ca_5Br(PO_4)_3$

M 565.2

Typical apatite-type struct. with P—O 153.1-154.8 pm, OPO 106.5-112.3°. Synth. from Calcium hydroxide phosphate ($Ca_5(OH)(PO_4)_3$), IC-016091 + HBr; or from Calcium phosphate ($Ca_3(PO_4)_2$), IC-016074 + $CaBr_2$ at 750-900° under N_2. Colourless hexagonal rods or plates. May show slight Br deficiency.

Klee, W.E. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 1837 (*synth, ir*)
Dykes, E., *Mater. Res. Bull.*, 1974, **9**, 1227 (*synth, cryst struct*)
Elliott, J.C. *et al, Acta Crystallogr., Sect. B*, 1981, **37**, 435 (*synth, cryst struct*)

BrCd$_5$O$_{12}$V$_3$ IC-001603

Cadmium bromide vanadate ($Cd_5Br(VO_4)_3$)

Cadmium vanadium bromide oxide ($Cd_5V_3BrO_{12}$), 11CI

[12394-00-2]

$Cd_5(VO_4)_3Br$

M 986.7

Apatite-like struct. with Br vacancies. *Cf* Cadmium iodide vanadate ($Cd_5I(VO_4)_3$), IC-016249; a Cl analogue is also known. Synth. by melting $Cd_3(VO_4)_2$ and excess $CdBr_2$ in a Pt crucible at 730-750°. The composition of the phase studied was $Br_{1.41}Cd_{4.86}O_{12}V_3$.

Engel, G., *Z. Anorg. Allg. Chem.*, 1968, **362**, 273 (*synth*)
Sundarsanan, K. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 3136 (*cryst struct*)
Wilson, A.J.C. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 3142 (*cryst struct*)
Baran, E.J. *et al, Rev. Chim. Minér.*, 1979, **16**, 527 (*ir*)
Wilson, A.J.C. *et al, Acta Crystallogr., Sect. A*, 1981, **37**, 441 (*struct*)

BrCl IC-001604

Bromine chloride (BrCl)

Bromine monochloride

[13863-41-7]

BrCl

M 115.3

Br—Cl 213.8 pm. Cannot be isolated free from bromine and chlorine. Mp −66°. Bp 5° dec. ΔH_f° +14.6 kJ mol^{-1}. Ir ν 440 cm^{-1}.

▷ EF9220000.

Vesper, H.G. *et al, J. Am. Chem. Soc.*, 1934, **56**, 620 (*synth, dissoc*)
Cole, L.G. *et al, J. Chem. Phys.*, 1952, **20**, 1543 (*uv*)
Stammreich, H. *et al, Spectrochim. Acta*, 1961, **17**, 1173 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 246 (*props*)

BrClFP IC-001605

Phosphorous bromide chloride fluoride, 9CI

Bromochlorofluorophosphine.
Bromochlorofluorophosphorus(III)

[20464-11-3]

PBrClF

M 165.3

(±)-*form*

Mp −122° to −120°. Disproportionates increasingly rapidly with rise in temp. above Mp.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 517 (*rev, bibl*)
Müller, A. *et al, Z. Naturforsch., B*, 1968, **23**, 588 (*raman*)
Montemayor, R.G. *et al, Inorg. Chem.*, 1973, **12**, 2482 (*synth, ir, ms, F-19 nmr, P-31 nmr*)

BrClHg IC-001606

Mercury bromide chloride (HgBrCl)

[13595-89-6]

HgBrCl

M 315.9

α-form contains regular distribution of Br and Cl; β-form random. Heating to Mp increases proportion of α-form. Crystallisation (from EtOH) increases proportion of β-form. Method of preparation and order of mixing anions affects the proportion of the two forms. Synth. from Hg_2Cl_2 and Br_2 or $HgCl_2$ and $HgBr_2$ at 90°. Cryst. Mp 240°.

Spiro, T.G. *et al, J. Am. Chem. Soc.*, 1961, **83**, 4305 (*uv, stability const*)
Marcus, Y. *et al, J. Phys. Chem.*, 1962, **66**, 1661 (*stability const*)
Eliezer, I., *J. Phys. Chem.*, 1964, **68**, 2722 (*stability const*)
Batsanov, S.S. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1965, 199 (*synth, thermal anal, powder struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1967, **B2**, 932 (*rev, bibl*)
Beattie, I.R. *et al, J. Chem. Soc. A*, 1970, 2433 (*raman, vapour*)
Malt'sev, A.A. *et al, Nature (London)*, 1971, **231**, 157 (*ir, vapour*)
Givan, A. *et al, J. Chem. Phys.*, 1976, **65**, 1851 (*ir, raman*)

Givan, A. *et al, J. Mol. Struct.*, 1978, **48**, 325 (*raman*)
Mehdi, S. *et al, J. Solid State Chem.*, 1981, **40**, 122 (*synth, thermal anal, powder struct, α-form, β-form*)

BrClI$^\ominus$ IC-001607

Bromochloroiodate(*I*)(1−)

[23297-41-8]

[Cl—I—Br]$^\ominus$

M 242.2 (ion)

Linear: I—Cl 284, I—Br 254 pm. Forms red salts. Dissociates in H_2O.

NH_4 salt: [16962-55-3].
Cs, K, Rb salts also known.

Me_4N salt: [15695-49-5].
Synth. from Me_4NBr and ICl in AcOH. Orange cryst. (AcOH and 3%ICl).

Wells, H.L. *et al, Am. J. Sci.*, 1892, **43**, 417 (*synth*)
Inorg. Synth., 1957, **5**, 167.
Migchelsen, T. *et al, Acta Crystallogr.*, 1967, **22**, 812 (*cryst struct, NH_4 salt*)
Maki, A.G. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 867 (*ir, raman*)
Dhamelincourt, P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1971, **272**, 50 (*ir, raman*)

BrClI$^\oplus$ IC-001608

Bromochloroiodine(1+), 11CI, 9CI

[Br—I—Cl]$^\oplus$

M 242.2 (ion)

Bent cation, spectroscopically characterised.

Hexachloroantimonate: [38656-80-3].
$BrCl_7ISb$ M 576.7
Synth. from $SbCl_5$, IBr and Cl_2. Large dark red cryst.

Fluorosulfate: [56244-21-4].
$BrClFIO_3S$ M 341.3
Synth. from a solid mixt. of IBr_2SO_3F and ICl_2SO_3F, heated to 95°. Crimson red solid. Mp 64-65°.

Shamir, J. *et al, Inorg. Chem.*, 1973, **12**, 1108 (*synth, raman, hexachloroantimonate*)
Wilson, W.W. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 665 (*fluorosulfate*)

BrClOS IC-001609

Thionyl bromide chloride

[22650-47-1]

O=SBrCl

M 163.4

Known only as a mixt. with $SOCl_2$ and $SOBr_2$. Synth. by reaction of $SOCl_2$ + KBr in liq. SO_2 at −30°.

Steudel, R. *et al, Z. Naturforsch., B*, 1969, **24**, 350 (*synth, ms, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 9, *Suppl. Vol.*, 1978, **1**, 71 (*bibl*)

BrClOSe IC-001610

Selenium bromide chloride oxide (SeBrClO), 11CI

Selenium oxy chloride bromide

[82735-17-9]

M 210.3 BrClSe=O

Formed by reaction by $OSeCl_2$ + $OSeBr_2$. Orange-red liq. Mp 17°.

Milne, J., *Spectrochim. Acta, Part A*, 1982, **38**, 569 (*synth, raman, Se-77 nmr*)

BrClO$_4$ IC-001611

Bromine(*I*) perchlorate 9CI, 8CI

[32707-10-1]

$BrOClO_3$

M 179.3

Synth. from $CsClO_4$ + $BrOSO_2F$ at −20°. Red liq., dec. at −20°. Mp −78°.

Schach, C.J. *et al, Inorg. Chem.*, 1971, **10**, 1078 (*synth, ir*)
Christe, K.O. *et al, Inorg. Chem.*, 1971, **10**, 1589 (*ir*)

BrClO$_6$ IC-001612

Bromyl perchlorate

Bromine(V) *oxide perchlorate* ($BrO_2(ClO_4)$)

[52225-67-9]

$O_2BrOClO_3$

M 211.3

Formed from pure O_3 + $BrOClO_3$ in CF_3Cl at −45°. Bright orange solid. Mp >-35° dec.

▷ Potentially explosive.

Schack, C.J. *et al, Inorg. Chem.*, 1974, **13**, 2378 (*synth, reactions*)

BrCl$_2^\ominus$ IC-001613

Dichlorobromate(*I*)(1−)

[14522-78-2]

[Cl—Br—Cl]$^\ominus$

M 150.8 (ion)

Linear centrosymmetric ion. Forms yellow-red salts. Dissociates in H_2O.

Me_4N salt: [1863-68-9].
Synth. from Me_4NBr and excess Cl_2 (g) in AcOH. Yellow cryst. Mp 160-163°.

Inorg. Synth., 1957, **5**, 167.
Evans, J.C. *et al, J. Chem. Phys.*, 1966, **44**, 4356 (*ir*)
Gabes, W. *et al, J. Mol. Struct.*, 1972, **14**, 267 (*struct*)

BrCl$_2$I$_2^\ominus$ IC-001614

Bromodichloroiodoiodate(1−)

[BrCl$_2$I$_2$]$^\ominus$

M 404.6 (ion)

Struct. not established.

Me_4N salt: [19510-32-8].
Synth. from $[Me_4N]ICl_2$ and ICl or from $[Me_4N]ICl_2$ and IBr. Red-brown cryst. Mp 24-25°. No evidence of isomerisation of pentahalide anion found.

2,2′-Bipyridinium(1+) salt: [23172-03-4].
Synth. from 2,2′-bipy.$HICl_2$ and IBr in 1,2-dichloroethane followed by dilution with CCl_4. Orange powder. Mp 67°.

Yoshiharu, Y. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 2223 (*synth, ir*)

IC-001615

$BrCl_3OP$

Phosphoryl bromide chloride ($POBrCl_2$), 9CI, 8CI

Bromodichlorophosphine oxide.
Bromodichlorooxophosphorus(V)

[13455-03-3]

$BrP(O)Cl_2$

M 197.7
Synth. from PCl_5 + PBr_5 + P_4O_{10}. Colourless liq. Fumes in moist air. d^{20} 2.09. Mp 10-11°. Bp 135°, Bp_{39} 52°. n_D^{20} 1.5092.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 516 (*rev, bibl*)
King, S.-T. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 1481 (*raman, ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 504, 1153 (*rev*)
Müller, A. *et al, Spectrochim. Acta, Part A*, 1973, **29**, 219 (*ir, raman*)
Grossmann, G. *et al, Z. Chem.*, 1976, **16**, 362 (*O-17 nmr*)

IC-001616

$BrCl_3O_8^{\ominus}$

Bis(perchlorato)bromate(*I*)(1−)

$[O_3Cl{-}O{-}Br{-}O{-}ClO_3]^{\ominus}$

M 278.8 (ion)
Cs salt: [51108-46-4].
$BrCl_2CsO_8$ M 411.7
Synth. from CsBr + Cl_2O_7 at −45°. Yellow solid, stable under dry N_2.

Christie, K.O. *et al, Inorg. Chem.*, 1974, **13**, 1452 (*synth, powder, struct, ir, raman*)

IC-001617

$BrCl_3P$

Phosphorus bromide chloride ($PBrCl_2$), 8CI

Phosphorous bromide dichloride, 9CI.
Bromodichlorophosphine. Bromodichlorophosphorus(III)

[13536-48-6]

$PBrCl_2$

M 181.7
Obt. only in mixt. with PBr_3Cl. Formed by equilibration between PCl_3 and PBr_3. Liq. Protonated by 'magic' acid. V. reactive to protic nucleophiles. Fumes in air. Bp 98-99°.

▷ Violent reaction to H_2O.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 514 (*rev, bibl*)
Müller, A. *et al, J. Mol. Struct.*, 1968, **2**, 149 (*ir, raman*)
Varmuza, K. *et al, Monatsh. Chem.*, 1971, **102**, 1037 (*synth, ms*)
Van de Griend, L.J. *et al, J. Am. Chem. Soc.*, 1975, **97**, 5958 (*synth, P-31 nmr*)
Gloede, J. *et al, Z. Anorg. Allg. Chem.*, 1981, **480**, 142 (*synth, P-31 nmr*)
Vengel'nikova, V.N. *et al, Zh. Obshch. Khim.*, 1982, **52**, 1318; *J. Gen. Chem. USSR (Engl. Transl.)*, 1982, **52**, 1160 (*synth, P-31 nmr*)

IC-001618

$BrCl_3Fe^{\ominus}$

Bromotrichloroferrate(*III*)(1−), 11CI

[31107-64-9]

$[FeBrCl_3]^{\ominus}$ (C_{3v})

M 242.1 (ion)
Mixed haloferrate from reaction of $FeCl_3$ with $Br^{\ominus}$. Salts are used in pesticides.

K salt: [93346-54-4]. *Iron(III) potassium bromide trichloride (FeKBrCl₃)*
$BrCl_3FeK$ M 281.2
Catalyst for bromination of styrene polymers.
Et_4N salt: [15651-10-2].
Synth. from $FeCl_3$ + $[Et_4N]Br$ in EtOH.
Ph_4P salt: [109740-51-4].
Catalyst for reaction of propylene oxide with amino acid derivs.

Clausen, C.A. *et al, Inorg. Chem.*, 1970, **9**, 220 (*ir, mössbauer, synth*)
Bhavsar, G.P. *et al, J. Mol. Struct.*, 1973, **16**, 343 (*ir*)

IC-001619

$BrCl_3P^{\oplus}$

Bromotrichlorophosphonium

Bromotrichlorophosphorus(I+), 9CI, 8CI

[36487-48-6]

$[PBrCl_3]^{\oplus}$

M 217.2 (ion)
Produced in ion-pairs with several anions, but few such salts isolated, although they may have been characterised spectroscopically in soln. Synth. from PCl_3 + Br_2 in Ac_2O or liq. HCl; or from PBr_3 + Cl_2 in oleum.

Tetrachloroborate: [16581-21-8].
$BBrCl_7P$ M 369.8
Synth. from PCl_3 + Br_2 in HCl(l) + BCl_3. White solid.
Hexafluorophosphate: [34269-62-0].
$BrCl_3F_6P_2$ M 362.2
Synth. from PCl_3 + Br_2 in HCl(l) + PCl_5. White solid.

Salthouse, J.A. *et al, J. Chem. Soc. A*, 1967, 1096 (*synth*)
Finch, A. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1863 (*synth, raman*)
Grimmer, A.-R., *Z. Anorg. Allg. Chem.*, 1973, **400**, 105 (*P-31 nmr*)
Malhotra, K.C. *et al, Aust. J. Chem.*, 1975, **28**, 991 (*formn, ir*)
Dillon, K.B. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1591 (*formn, P-31 nmr*)
Dillon, K.B. *et al, Polyhedron*, 1983, **2**, 641 (*formn, P-31 nmr*)

IC-001620

$BrCl_3Si$

Bromotrichlorosilane

Silicon bromide chloride ($SiBrCl_3$). Silicon bromide trichloride

[13465-74-2]

$SiBrCl_3$ (C_{3v})

M 214.3
Colourless liq. d 1.826. Mp −62°. Bp 80.3°. Dec. in H_2O.

Niemann, U. *et al, Z. Naturforsch., A*, 1971, **26**, 547 (*ir*)
Bevan, W.I., *J. Chem. Soc., Dalton Trans.*, 1974, 2305.
Hass, D. *et al, Z. Chem.*, 1975, **15**, 240 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 680 (*synth*)
Voronkov, M.G. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **232**, 817 (*ir*)
Sladkov, I.B. *et al, Zh. Fiz. Khim.*, 1982, **56**, 1032.

IC-001621

$BrCl_3Sn$

Bromotrichlorostannane

Tin bromide chloride ($SnBrCl_3$). Tin bromide trichloride

[13536-50-0]

$SnBrCl_3$ (C_{3v})

M 304.9
Colourless liq. d^{13} 2.51. Mp −31°. Bp_{30} 50°.

Cerf, C. *et al, Bull. Soc. Chim. Fr.*, 1964, 389, 2818 (*ir*)

Shult, D.E., *Diss. Abstr. Int., B*, 1977, **38**, 187.
Motsarev, G.V. *et al, Zh. Obshch. Khim.*, 1977, **47**, 379 (*synth*)
Colton, R. *et al, Inorg. Chim. Acta*, 1982, **61**, 1 (*Sn-119 nmr*)

IC-001622

$BrCl_4H_2OPt^{\ominus}$

Aquabromotetrachloroplatinate(*IV*)(1−), 10CI

[65176-63-8]

$[(H_2O)PtBrCl_4]^{\ominus}$

M 434.8 (ion)
Not isol. Prep. *in situ* for kinetic substitution studies by Br_2 + $[PtCl_4]^{2\ominus}$ in H_2O. Isomerism not investigated.

Elding, L.I. *et al, Inorg. Chim. Acta*, 1977, **24**, 239.

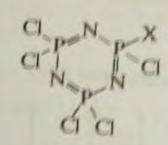
IC-001623

$BrCl_5N_3P_3$

2-Bromo-2,4,4,6,6,6-pentachloro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 8CI

Bromopentachlorocyclotriphosphonitrile.
Bromopentachlorocyclotriphosphazene. 2-Bromo-2,4,4,6,6-pentachloro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2-Bromo-2,4,4,6,6-pentachloro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine

[14740-93-3]



X = Br

M 392.1
Formed from mixture of $P_3N_3Cl_6$ and $P_3N_3Br_6$ heated to 250°. Orthorhombic cryst. Mp 122° (120°).

Rotzsche, H. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 687 (*synth, gc*)
Engelhardt, G. *et al, Z. Naturforsch., B*, 1966, **21**, 1231 (*P-31 nmr*)
Coxon, G.E. *et al, Inorg. Chim. Acta*, 1967, **1**, 381 (*synth, ir*)
Stahlberg, U. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 2057, 2691 (*ir, raman*)
Lakatos, B. *et al, Acta Chim. (Budapest)*, 1969, **60**, 303 (*synth, uv*)
Coxon, G.E. *et al, J. Chem. Soc. A*, 1969, 358 (*ms*)

IC-001624

$BrCl_5Nb^{\ominus}$

Bromopentachloroniobate(*V*)(1−), 11CI

[34373-30-3]

$[NbBrCl_5]^{\ominus}$ (C_{4v})

M 350.0 (ion)
Octahedral anion.

H compd.: [98538-82-0].
$BrCl_5HNb$ M 351.0
Synth. by dissolving $NbCl_5$ in Et_2O saturated with HBr. Deep red solid + $2Et_2O$.
Et_4N salt: [23081-23-4].
Synth. from a stoichiometric mixture of $NbCl_5$ and $[Et_4N]Br$ in MeCN. Pale yellow solid.

Ozin, G.A. *et al, J. Chem. Soc. A*, 1969, 642 (*synth, ir, uv-vis*)
Kolditz, L. *et al, Z. Anorg. Allg. Chem.*, 1970, **376**, 1 (*synth*)
Papadimitriou, C. *et al, J. Less-Common Met.*, 1985, **108**, 217 (*synth, ir*)

IC-001625

$BrCl_5Os^{2\ominus}$

Bromopentachloroosmate(*IV*)(2−)

[16920-00-6]

$[OsCl_5Br]^{2\ominus}$

M 447.3 (ion)
Usually obt. in soln. for studies of substn. kinetics. All the species $[OsCl_{6-n}Br_n]^{2\ominus}$ are known.

Joergensen, C.K. *et al, Z. Naturforsch., A*, 1967, **22**, 945 (*uv*)
Mueller, H., *Fresenius' Z. Anal. Chem.*, 1969, **247**, 145; 1983, **314**, 758 (*tlc, hplc*)
Preetz, W. *et al, Z. Anorg. Allg. Chem.*, 1974, **407**, 1; 1976, **420**, 97; 1981, **479**, 7 (*synth, uv, ir, kinetics*)
Urushiyama, A., *Chem. Lett.*, 1976, 1409 (*uv*)
Zerbe, H.D. *et al, Z. Anorg. Allg. Chem.*, 1981, **479**, 17 (*kinetics*)

IC-001626

$BrCl_5Re^{2\ominus}$

Bromopentachlororhenate(*IV*)(2−), 10CI

$[ReBrCl_5]^{2\ominus}$

M 443.3 (ion)
Di-K salt: [63701-67-7].
$BrCl_5K_2Re$ M 521.5
Formed by fusion of K_2ReBr_6 and K_2ReCl_6 above 420°. Separated from other mixed ions by ion column chromatography and extracted by tridodecylamine in Et_2O. Solid. Distorted K_2PtCl_6-type structure.

Hauck, J. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2124 (*synth, cryst struct, ir, props*)
Mueller, H. *et al, Z. Anorg. Allg. Chem.*, 1983, **503**, 15 (*synth, cryst struct, uv, props*)

IC-001627

$BrCl_5Ta^{\ominus}$

Bromopentachlorotantalate(*V*)(1−), 11CI

$[TaBrCl_5]^{\ominus}$ (C_{4v})

M 438.1 (ion)
Octahedral anion. A wide range of mixed halides $[TaX_5Y]^{\ominus}$ is known.

H compd.: [98538-83-1].
$BrCl_5HTa$ M 439.1
Synth. as an $(Et_2O)_2H$ salt by adding $TaCl_5$ to a saturated soln. of HBr in Et_2O. Yellow-orange hygroscopic solid + Et_2O. Sol. DMF; sl. sol. MeCN, Me_2CO, alcohols. The Et_2O may be replaced by Py or ethylenediamine.
Et_4N salt: [22602-30-8].
Synth. from $[Et_4N]Br$ and $TaCl_5$ in MeCN or $MeCN/CHCl_3$. Pale yellow solid.
Hexakis(acetonitrile)copper(2+) salt: [69569-65-9].
$C_{12}H_{18}Br_2Cl_{18}CuN_6Ta$ M 1005.1
Synth. from $CuBr_2$ and $TaCl_5$ in MeCN. Similar salts known for several first row transition metals.

Ozin, G.A. *et al, J. Chem. Soc. A*, 1969, 642 (*synth, uv-vis, ir, raman*)
Kolditz, L. *et al, Z. Anorg. Allg. Chem.*, 1970, **376**, 1 (*synth*)
Masaguer, S. *et al, Acta Cient. Compostelana*, 1978, **15**, 3 (*synth, ir, M(MeCN)₆²⁰ salts*)
Papadimitriou, C. *et al, J. Less-Common Met.*, 1985, **108**, 217 (*synth, ir, H compd*)

IC-001628

$BrCl_5P_2$

Phosphorus bromide chloride (P_2BrCl_5), 9CI

Bromononachlorodiphosphorus(V)

[53096-45-0]

$[PCl_4^{\oplus}]_6[PCl_3Br^{\oplus}]_2[PCl_6^{\ominus}]_4[Br^{\ominus}]_4$ (hexamer)

M 460.9
Exists as ionic hexamer.

Bis(bromotrichlorophosphonium) hexakis(tetrachlorophosphonium) tetrakis(hexachlorophosphate)

Hexameric-form

$Br_4Cl_{36}P_{12}$ M 2765.5

Synth. from PCl_5 + Br_2 in $AsCl_3$. Pale yellow cryst. V. hygroscopic. Dec. at 142°.

Kolditz, L. et al, Z. Anorg. Allg. Chem., 1957, 293, 286 (synth)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 515 (rev, bibl)
Bentley, F.F. et al, J. Inorg. Nucl. Chem., 1974, 36, 457 (synth, ir, raman, P-31 nmr, struct)

$BrCoH_{15}N_5^{2\oplus}$ IC-001629

Pentaamminebromocobalt(*III*)(2+), 10Cl, 11Cl

[14970-15-1]

$[Co(NH_3)_5Br]^{2\oplus}$

M 223.9 (ion)
Many salts studied. Aquation, photolysis and reduction much studied.

Dibromide: [14283-12-6].
$Br_2CoH_{15}N_5$ M 383.7
Fine light lavender-coloured cryst. or large purple cryst. Photolysis suggests production of Co(*II*) and Br radicals. Dec. at 100° *in vacuo*.

Dichloride: [13601-38-2].
Cryst. (H_2O, pH 4). Dec. at 110° *in vacuo*.

Diiodide: Garnet coloured transparent thick plates. Dec. at 40° *in vacuo*.

Diperchlorate: [14591-65-2].
Violet prisms.

Ephraim, F. et al, Chem. Ber., 1923, 56, 1531 (synth, salts)
Inorg. Synth., 1939, 1, 186 (synth)
Woodhouse, W.W. et al, J. Inorg. Nucl. Chem., 1963, 25, 843 (thermal dec)
Sazzora, L. et al, Inorg. Chem., 1964, 3, 1772 (ir)
Penhale, S.A. et al, J. Am. Chem. Soc., 1965, 87, 2514 (photol)
Kirk, A.D. et al, J. Phys. Chem., 1983, 87, 3108 (photochem)
Nakashima, Y. et al, Bull. Chem. Soc. Jpn., 1989, 62, 2455 (N-15 nmr)

$BrCrH_{15}N_5^{2\oplus}$ IC-001630

Pentaamminebromochromium(*III*)(2+), 11Cl, 10Cl, 9Cl

Bromopentaamminechromium(III)

[22269-65-2]

$[CrBr(NH_3)_5]^{2\oplus}$

M 217.0 (ion)
Octahedral cation.

Dibromide: [13601-60-0]. *Chromium(III) bromide pentaammine*
Synth. from $[Cr(OH_2)(NH_3)_5](ClO_4)_2$ and aq. $HClO_4$/NaBr at 50°. Reddish solid. Dec. by H_2O.

Diperchlorate: [60551-54-4].
Obt. by metathesis of the bromide.

Inorg. Synth., 1957, 5, 134 (synth)
Garner, C.S. et al, Transition Met. Chem., 1970, 6, 59 (rev)
Brauer, G., Handbuch Präp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 3, 1498 (synth, bromide)
Andrianov, V.T.M. et al, Inorg. Chem., 1976, 15, 2044 (cryst)
Ramasami, T. et al, Inorg. Chem., 1976, 15, 2885 (synth, equation)
Ueno, H. et al, Bull. Chem. Soc. Jpn., 1981, 54, 1821 (thermal dec)
Ue, N. et al, J. Phys. Chem., 1982, 86, 1694 (equation)

$BrCrO_3^{\ominus}$ IC-001631

Bromotrioxochromate(1−), 9Cl

Bromochromate

[33091-56-4]

$[CrO_3Br]^{\ominus}$

M 179.8 (ion)
Prepd. by reaction of CrO_3 with HBr.

Rb salt: [39043-67-9].
$BrCrO_3Rb$ M 265.3
Yellow cryst.

Cs salt: [39043-68-0].
$BrCrCsO_3$ M 312.8
Yellow cryst.

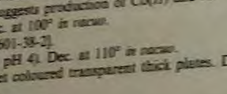
Pyridinium salt: [107139-14-0]. *Pyridinium bromochromate*
Reagent for bromination and oxidation of org. compds. Dark brown cryst.

[20860-99-5, 54678-82-9, 99921-38-7]

Koeniger-Ahlborn, E. et al, Z. Naturforsch., B, 1972, 27, 1108 (synth, ir, uv)
Mueller, A. et al, Spectrochim. Acta, Part A, 1973, 29, 1773 (ir, raman)
Narayanan, N. et al, Indian J. Chem., Sect. B, 1986, 25, 228 (synth, use, pyridinium salt)

$BrCrO_5^{\ominus}$ IC-001632

Bromooxodiperoxychromate(*VI*)(1−), 8Cl



X = Br

M 211.8 (ion)
Distorted pentagonal pyramidal struct. proposed.

$MeAsPh_3$ salt: [21005-03-8].
Blue cryst. Stable for several months. Dec. at 110°.

Armstrong, R. et al, Aust. J. Chem., 1968, 21, 897 (synth, ir)
Sastri, M.N. et al, J. Inorg. Nucl. Chem., 1968, 30, 1727 (synth, props)

BrCs IC-001633

Caesium bromide (CsBr), 8Cl

[7787-69-1]

CsBr

M 212.8
CsCl type struct. Prepd. by slow neutralisation of Cs_2CO_3 with HBr in aq. soln. Alternatively reaction of Cs_2CO_3 with Br_2 in aq. soln. containing $N_2H_4.H_2O$ affords pure CsBr. Commercially available. Used in optical windows. Deliquescent colourless cubic cryst. V. sol. H_2O (124 g per 100 cm^3 at 25°). Mp 636°. Bp 1300°. ΔH_f° −406 kJ mol^{-1}; ΔG_f° −391 kJ mol^{-1}; S° 113 J K^{-1} mol^{-1}.

▷ Irritant. FK9275000.

Sigma-Aldrich Library of Chemical Safety Data, 2, 715C.
Davey, W.P., Phys. Rev., 1923, 21, 143 (cryst struct)
Gmelin Handbook Inorg. Chem., Syst. No. 25, 1955, 171 (rev, bibl)
Yulich, A.I. et al, Promst. Khim. React. Osobo Chist. Veshchestv., 1967, 40; CA, 1969, 70, 53444 (synth)
Mooibroek, S. et al, J. Magn. Reson., 1986, 66, 542 (Cs-133 nmr)
Merck Index, 11th Ed., 1989, No. 2002.

$BrCsO_3$ IC-001634

Caesium bromate(*V*) ($CsBrO_3$)

Bromic acid, caesium salt, 8Cl

[13454-75-6]

$CsBrO_3$

M 260.8
Prepd. by dissolving crystalline Cs_2CO_3 in aq. $HBrO_3$. Colourless cryst. (H_2O). Dec. on heating to form CsBr and O_2. Radiolysis results in formation of $BrO^{\ominus}$, and $O_3^{\ominus}$ and enhanced thermal dec. Spar. sol. H_2O (3.7 g per 100 cm^3 at 25°). Mp ~420°. ΔH_f° −366 kJ mol^{-1}.

Schawlow, A.L., J. Chem. Phys., 1954, 22, 1211 (Br-81 nqr)
Gmelin Handbook Inorg. Chem., Syst. No. 25, 1955, 2, 188 (rev, bibl)
Bancroft, G.M. et al, J. Inorg. Nucl. Chem., 1965, 27, 1545 (thermal dec)
Shklovskaya, R.M. et al, C.A., 1968, 69, 48786 (synth)
Shklovskaya, R.M. et al, Zh. Prikl. Khim. (Leningrad), 1969, 42, 288 (purif)
Boyd, G.E. et al, J. Phys. Chem., 1970, 74, 3490 (radiolysis)
Kondilenko, I.I. et al, Opt. Spektrosk., 1975, 38, 689 (raman)
Masaguer, J.R. et al, J. Chem. Thermodyn., 1976, 8, 519 (thermochem data)
Weiden, N. et al, J. Mol. Struct., 1980, 58, 43 (O-17, Cs-137 nqr)
Mohanty, S.R. et al, Radiochem. Radioanal. Lett., 1980, 42, 31 (radiolysis, thermal dec)

BrCu IC-001635

Copper bromide (CuBr)

Cuprous bromide

[7787-70-4]

CuBr

M 143.4
Polymorphic. γ-CuBr (zinc-blende struct.) exists below 390°, β-CuBr (Wurtzite struct.) between 391 and 470°, and α-CuBr (cubic) above 470°. Prepd. by reducing aq. $CuSO_4$ contains KBr with SO_2 or with metallic Cu. Can also be prepd. from the elements. Catalyst in org. synth. Colourless cryst. Sl. sol. H_2O; prac. insol. Me_2CO. Mp 504°. Bp 1345°.

Krug, J. et al, Z. Naturforsch., A, 1952, 7, 369 (cryst struct, polymorphism)
Rosenstock, H.M. et al, J. Chem. Phys., 1955, 23, 2442 (ms)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, 1, 165 (use)
Brauer, G., Handbuch Präp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 973 (synth)
Becker, K.D., J. Chem. Phys., 1978, 68, 3785 (nmr)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 7, 103 (rev)
Theis, A.B. et al, Synth. Commun., 1981, 11, 157 (synth)
Merck Index, 11th Ed., 1989, No. 2666.

BrF IC-001636

Bromine fluoride (BrF)

Bromine monofluoride

[13863-59-7]

BrF

M 98.9
Brominating agent. Red-brown gas, dec. at r.t. Mp −33°. Bp 20°. ΔH_f° −58.6 kJ mol^{-1}.

Dutie, R.A. et al, J. Phys. Chem., 1952, 56, 316 (uv)
Stein, L., Halogen Chem., (Gutmann, V., Ed.) Academic Press, London, 1967, 151 (rev)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 4, 246 (props)
Buerger, H. et al, Z. Naturforsch., A, 1986, 41, 1015 (ir)
Rozen, S. et al, J. Chem. Soc., Chem. Commun., 1987, 752 (synth, use)

BrFHg IC-001637

Mercury bromide fluoride (HgBrF)

[56564-54-6]

HgBrF

M 299.4
Synth. from Hg_2F_2 and Br_2 or from condensed HgF_2 and $HgBr_2$ vapour. White cryst. at r.t., turns yellow on standing; yellow cryst. at 90°. Dec. at 184° → HgF_2 + $HgBr_2$.

Jander, G. et al, Z. Anorg. Allg. Chem., 1951, 265, 117 (synth)
Rastogi, R.P. et al, J. Inorg. Nucl. Chem., 1975, 37, 1167 (synth, powder struct)
Girvan, A. et al, J. Chem. Phys., 1978, 68, 5653; 1980, 72, 3809 (ir, raman)

$BrFI^{\ominus}$ IC-001638

Bromofluoroiodate(1−), 11Cl, 10Cl, 9Cl

[19236-17-0]

$[BrIF]^{\ominus}$

M 225.8 (ion)

Cs salt: [75374-90-2].
Synth. from CsF and excess IBr at 50° under dry N_2.

Tl salt: [55482-13-8].
Synth. from TlF and IBr under vacuum at 80-85°.

Batsanov, S.S. et al, Zh. Neorg. Khim., 1975, 20, 689; Russ. J. Inorg. Chem. (Engl. Transl.), 1975, 20, 464 (synth Tl salt)
Birchall, T. et al, J. Chem. Soc., Dalton Trans., 1980, 1060 (mössbauer, synth, Cs salt)

BrFOS IC-001639

Thionyl bromide fluoride

Sulfur(IV) bromide fluoride oxide (SBrFO)

[81539-20-0]

O=SBrF

M 146.9
Synth. by reaction of $SOBr_2$ + F_2.

Gmelin Handbook Inorg. Chem., Syst. No. 9, 1978, B1 (bibl)
Rappert, I., J. Fluorine Chem., 1982, 20, 75 (synth, F-19 nmr)

$BrFO_2$ IC-001640

Bromine fluoride oxide ($BrFO_2$), 9Cl

Bromyl fluoride, 10Cl

[22585-64-4]

M 130.9
Square pyramidal monomer. Synth. from $KBrO_3$ and BrF_3 in HF at −50°. White solid at low temp. Sol. BrF_3. Mp −10°.

[64544-65-6, 67452-70-4]

Sloth, E.N., J. Phys. Chem., 1969, 73, 1569 (ms)
Gillespie, R.J. et al, J. Chem. Soc., Dalton Trans., 1977, 1539 (synth, raman, F-19 nmr)
Jacob, E., Z. Anorg. Allg. Chem., 1977, 433, 255 (synth, ir)
Christie, K.O. et al, Inorg. Chem., 1978, 17, 2744 (ir)

$BrFO_2S$ IC-001641

Sulfuryl bromide fluoride, 10CI

Sulfonyl bromide fluoride

[13536-61-3]

$S(O)_2BrF$

M 162.9

Tetrahedral molecule. Synth. from BrF + SO_2. Thermally stable colourless liq., rapidly hydrol. d^0 2.17. Mp −86°. Bp 40°.

▷ Reacts slowly with glass.

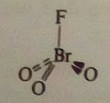
Jolly, W.C., *Prep. Inorg. React.*, 1966, **3**, 35 (*rev, ir, nmr*)
Radley, J. *et al*, *J. Mol. Spectrosc.*, 1973, **48**, 100 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 192 (*synth*)

$BrFO_3$ IC-001642

Bromine fluoride oxide ($BrFO_3$), 9CI

Perbromyl fluoride, 9CI

[37265-91-1]



M 146.9

Tetrahedral molecule isostructural with ClO_3F. Synth. from $KBrO_4$ and SbF_5 in anhydrous HF. Highly volatile liq. or gas; often yellow due to impurities. Hydrol. in alkaline solns. Mp −110°.

[25251-03-0]

Appelman, E.H. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 4561 (*synth, ms*)
Claassen, H.H. *et al*, *Inorg. Chem.*, 1970, **9**, 622 (*struct, raman*)
Johnson, G.K. *et al*, *Inorg. Chem.*, 1972, **11**, 800 (*thermodynamics*)
Appelman, E.H. *et al*, *J. Mol. Struct.*, 1976, **35**, 139 (*struct*)

$BrFO_3S$ IC-001643

Bromine(*I*) fluorosulfate (Br(SFO$_3$)), 11CI, 10CI, 9CI

[13997-93-8]

$BrOS(O)_2F$

M 178.9

Formed by thermal dec. of Bromine(*III*) fluorosulfate, IC-001656. V. readily hydrol. red-brown liq. d^{25} 2.238. Mp −31.5°. Bp 117.3°.

Roberts, J.E. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 352 (*synth, props*)
Hohorst, F.A. *et al*, *Inorg. Chem.*, 1966, **5**, 2069 (*F-19 nmr*)
Aubke, F. *et al*, *Inorg. Chem.*, 1968, **7**, 599 (*synth*)
Woolf, A.A., *New Pathways in Inorg. Chem.*, Ebsworth, E.A.V., *et al*, Eds., 1968, 327 (*rev*)
Johri, K.K. *et al*, *J. Fluorine Chem.*, 1982, **19**, 227 (*reactions*)

BrFPb IC-001644

Lead(*II*) bromide fluoride (PbBrF), 9CI

[13569-42-1]

PbBrF

M 306.1

Has a layer struct. Formed when Pb salt is added to a soln. containing both $Br^{\ominus}$ and $F^{\ominus}$. Solid. Spar. sol. H_2O.

Talipov, Sh.T. *et al*, *CA*, 1959, **53**, 13736g (*sol'y*)

Rulmont, A., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1973, **276**, 775 (*synth, cryst struct*)
Rulmont, A., *Spectrochim. Acta, Part A*, 1974, **30**, 161 (*ir, raman*)

$BrF_2^{\ominus}$ IC-001645

Bromofluorofluorate

$[BrFF]^{\ominus}$

M 117.9 (ion)

Synth. from MBr and F_2/Ar. Characterised by ir at 15K in an Ar matrix.

K salt: [69204-10-0].
Rb salt: [69204-11-1].
Cs salt: [69204-12-2].

Miller, J.H. *et al*, *Inorg. Chem.*, 1979, **18**, 988 (*ir*)

$BrF_2^{\ominus}$ IC-001646

Difluorobromate(1−), 11CI, 10CI, 9CI

[25730-96-5]

$[F—Br—F]^{\ominus}$

M 117.9 (ion)

Linear symmetric anion. Synth. from MBr and F_2/Ar.

Na salt: [69204-01-9].
K salt: [69204-02-0].
Rb salt: [69204-03-1].
Cs salt: [40419-00-9].

Complicated synth. from BrF_3 in Br_2 and CsF. Light yellow powder.

Surles, T. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 668 (*synth, raman, Cs salt*)
Zakzhevskii, *et al*, *Zh. Strukt. Khim.*, 1976, **17**, 763; *J. Struct. Chem. USSR (Engl. Transl.)*, 1976, **17**, 659 (*theory*)
Miller, J.H. *et al*, *Inorg. Chem.*, 1979, **18**, 988 (*ir*)
Kirillov, Y.B. *et al*, *Zh. Strukt. Khim.*, 1980, **21**, 9 (*theory*)
Jacox, M.E., *J. Phys. Chem. Ref. Data*, 1984, **13**, 945.

$BrF_2^{\oplus}$ IC-001647

Difluorobromine(1+)

[31159-95-2]

$[F—Br—F]^{\oplus}$

M 117.9 (ion)

Bent ion. Angle 90.7°, Br—F 172 pm. Colourless ion. Reacts violently with H_2O.

Hexafluoroarsenate: [30051-24-2].

Synth. from BrF_3 and AsF_5. White cryst. Marginally stable at r.t.

Hexafluoroantimonate: [19379-47-6].

BrF_6Sb M 353.6

Synth. from BrF_3 and SbF_5. White cryst., developing pink to red colour on storage.

Hexafluorogermanate(2−) (2:1): [30051-23-1].

$Br_2F_{10}Ge$ M 422.4

Synth. from GeF_4 and BrF_3. White cryst. Subl. 20° *in vacuo*.

Edwards, A.J. *et al*, *J. Chem. Soc. A*, 1969, 1467 (*struct*)
Christie, K.O. *et al*, *Inorg. Chem.*, 1970, **9**, 2296 (*ir, raman, synth*)
Surles, T. *et al*, *Inorg. Chem.*, 1971, **10**, 611 (*raman*)
Richards, G.W. *et al*, *J. Fluorine Chem.*, 1971, **1**, 129 (*heat of formation*)
Gillespie, R.J. *et al*, *Advan. Raman Spectrosc.*, 1972, **1**, 539 (*raman*)
Surles, T. *et al*, *J. Fluorine Chem.*, 1973, **3**, 453 (*raman*)
Edwards, A.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 175 (*cryst struct, hexafluorogermanate*)

Cyr, T. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 2143 (*F-19 nmr*)
Mitkin, V.N. *et al*, *Koord. Khim.*, 1983, **9**, 20 (*F-19 nmr, struct*)
Popov, A.I. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **576**, 242 (*synth*)

$BrF_2NO_4S_2$ IC-001648

N-Bromoimidodisulfuryl fluoride, 9CI

N-Bromoiminodisulfonyl difluoride

[104715-40-4]

$BrN(SO_2F)_2$

M 260.0

Synth. from $BrOSO_2F$ + $Hg[N(SO_2F)_2]_2$ at 22°. Pale yellow liq., stable in the dark. Mp −19°. Forms BrCl with AgCl.

Singh, S. *et al*, *Inorg. Chem.*, 1986, **25**, 4596 (*synth, ir, ms, F-19 nmr*)

BrF_2NS IC-001649

Bromoimidosulfurous difluoride, 11CI

[25005-08-7]

$BrN{=}SF_2$

M 163.9

Formed from $Hg(NSF_2)_2$ + Br_2. Light-sensitive, pale-yellow liq. Low thermal stability. Bp 56.5°. Can be stored in glass containers at −78°.

▷ Toxic, reacts explosively with H_2O.

Inorg. Synth., 1986, **24**, 20 (*synth, ir, F-19 nmr*)

BrF_2OP IC-001650

Phosphoryl bromide fluoride ($POBrF_2$), 9CI, 8CI

Bromodifluorophosphine oxide.
Bromodifluorooxophosphorus(V)

[14014-18-7]

$BrP(O)F_2$

M 164.8

Synth. from Diphosphoryl fluoride, IC-018436 + PBr_5, or from Phosphorodifluoridic acid, IC-018146 + PBr_5. Volatile liq. Fumes in air. d_4^{20} 2.001, d^0 2.099 (liq.). Mp −84.8°. Bp 30.5°. ΔH_f°(g) −957 kJ mol^{-1}.

▷ Reacts violently with H_2O.

Booth, H. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 3120 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 510 (*rev, bibl*)
Müller, A. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1967, **71**, 571 (*ir, raman*)
Müller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **350**, 246 (*F-19 nmr, P-31 nmr*)
Roesky, H.W., *Chem. Ber.*, 1968, **101**, 636 (*synth*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 455, 1153 (*rev*)
Inorg. Synth., 1974, **15**, 194 (*synth*)
Binneweis, M. *et al*, *Thermochim. Acta*, 1986, **103**, 401 (*ms*)

BrF_2P IC-001651

Phosphorus bromide fluoride ($PBrF_2$), 8CI

Phosphorous bromide difluoride, 9CI.
Bromodifluorophosphine. Bromodifluorophosphorus(III)

[15397-40-7]

$PBrF_2$

M 148.8

Monomeric. Synth. from PBr_3 + SbF_3; or from Et_2NPF_2 + PBr_3. Gas. Best synth. immediately before use. Reacts slowly with Hg. Fumes in air. Mp −133.8°. Bp −16.1°.

▷ Sharp odour.

BH_3 complex (1:1):

$BBrF_2H_3P$ M 162.7

V. volatile liq. Mp −125°. Bp 23.7°.

Booth, H.S. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 2934 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 509 (*rev, bibl*)
Inorg. Synth., 1967, **10**, 147 (*synth, ir*)
Müller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **350**, 256 (*ir, F-19 nmr, P-31 nmr*)
Paine, R.T. *et al*, *Inorg. Chem.*, 1972, **11**, 1237 (*complex, ms, ir, pmr, B-11 nmr, F-19 nmr, P-31 nmr*)
Morse, J.G. *et al*, *J. Chem. Phys.*, 1972, **57**, 5372 (*struct*)
Cradock, S. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 940 (*pe*)
Odom, J.D. *et al*, *Inorg. Chem.*, 1980, **19**, 2651 (*complex, pmr, B-11 nmr, F-19 nmr, P-31 nmr*)
Albers, W. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1985, **15**, 187 (*synth*)

BrF_2PS IC-001652

Thiophosphoryl bromide fluoride ($PSBrF_2$), 9CI, 8CI

Bromodifluorophosphine sulfide.
Bromodifluorothioxophosphorus(V)

[13706-09-7]

$BrP(S)F_2$

M 180.9

Interatomic distances (vap.): P═S 188.1, P—F 154.3, P—Br 215.5 pm; angles: FPF 98.3°, SPF 118.2°, SPBr 118.2°. Synth. from $PSBr_3$ + SbF_3. Colourless volatile liq. d^0 1.94. Mp −136.9°. Bp 35.5°.

▷ XN2985000.

Booth, H.S. *et al*, *J. Am. Chem. Soc.*, 1943, **65**, 1834 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 601 (*rev, bibl*)
Müller, A. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1967, **71**, 571 (*ir, raman*)
Müller, A. *et al*, *Mol. Phys.*, 1968, **14**, 591 (*F-19 nmr, P-31 nmr*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 534, 1153 (*rev*)
Müller, A. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 219 (*ir, raman*)
Elbel, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1762 (*pe*)
Acha, L. *et al*, *J. Mol. Struct.*, 1981, **73**, 111 (*ed, struct*)

BrF_3 IC-001653

Bromine fluoride (BrF_3)

Bromine trifluoride

[7787-71-5]

BrF_3

M 136.8

T-shaped molecule. Outer bond lengths 181.0 pm, stem 172.1 pm. Angle 86.2°. Commercially available. Used as a powerful fluorinating agent and in nuclear fuel processing. Straw-coloured liq. d_4^{20} 2.843. Mp 8.8°. Bp 127°. ΔH_f° −301 kJ mol^{-1}.

▷ V. corrosive. Reacts violently with H_2O, organic materials. EF9360000.

Inorg. Synth., 1950, **3**, 184 (*synth*)
Haendler, H.M. *et al*, *J. Chem. Phys.*, 1954, **22**, 1939 (*ir*)
Irsa, A.P. *et al*, *J. Inorg. Nucl. Chem.*, 1958, **6**, 77 (*ms*)
Muetterties, E.L. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 1084 (*F-19 nmr*)

Stein, L., *Halogen Chem.*, (Gutmann, V., Ed.) Academic Press, London, 1967, 155 (*rev*)
Davis, R.A. *et al*, *J. Org. Chem.*, 1967, **32**, 3478 (*use*)
Inorg. Synth., 1970, **12**, 233 (*handling and disposal*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 246 (*props*)

BrF_3H_4NSb IC-001654

Ammonium bromotrifluoroantimonate(1−), 10CI
Bromotrifluoroantimonate(III) *ammonium salt*
[61392-34-5]

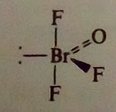
$NH_4[SbBrF_3]$

M 276.6
Synth. from SbF_3 + NH_4Br in aq. soln. Orthorhombic plates.

Ducourant, B. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1976, **283**, 203 (*synth, cryst struct*)
Birchall, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 131 (*mössbauer*)
Zemnukhova, L.A. *et al*, *Zh. Fiz. Khim.*, 1979, **53**, 48; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1979, **53**, 26 (*synth, nqr*)

BrF_3O IC-001655

Bromine(*V*) fluoride oxide (BrF_3O), 11CI
Bromine oxide trifluoride
[61519-37-7]



M 152.8
Synth. from $K[BrOF_4]$ + $O_2[AsF_6]$ in BrF_5. Colourless liq. Stable at 20°. Rapidly hydrol. by H_2O. Associated as liq. (Vp < 5 mm at 25°).

Bougon, R. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1976, **283**, 461 (*synth, raman*)
Holloway, J.H. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1983, **27**, 179 (*rev*)

$BrF_3O_9S_3$ IC-001656

Bromine(*III*) fluorosulfate
Bromine tris(fluorosulfate)
[29880-59-9]

$Br[OS(O)_2F]_3$

M 377.0
Synth. from Br_2 + $(FSO_2O)_2$. Pale yellow solid, stable at 20°. Vigorously hydrol. to Br_2 + O_2 + $HOSO_2F$. Mp 59°.

Roberts, J.E. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 352 (*synth*)
Jolly, W.L., *Prep. Inorg. React.*, 1966, **3**, 35 (*rev*)
Aubke, F. *et al*, *Inorg. Chem.*, 1968, **7**, 599 (*synth*)
Carter, H.A. *et al*, *Inorg. Chem.*, 1970, **9**, 2485 (*raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 341 (*synth*)

$BrF_4^{\ominus}$ IC-001657

Tetrafluorobromate(*III*)(1−)
[19702-38-6]

$[BrF_4]^{\ominus}$

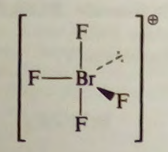
M 155.8 (ion)
Square-planar; Br—F 189 pm.
▷ Reacts violently with H_2O.

Rb salt: [16060-02-9].
BrF_4Rb M 241.3
Colourless solid. Dec. on heating.
Cs salt: [15705-88-1].
$BrCsF_4$ M 288.8
Synth. under vacuum from CsF and BrF_3 at 80°.
Colourless solid. Dec. on heating.
Ag salt: [35967-89-6].
$AgBrF_4$ M 263.7
Synth. from BrF_3 and Ag or Ag_2CO_3.
Nitrosyl salt:
BrF_4NO M 185.9
Synth. from BrF_3 and NOF at r.t. White cryst. Subl. 100° (in N_2). Dec. at 24.8° (2 mm Hg).
Me_4N salt: [122821-60-7].
Hazardous synth. from $[Me_4N]F$ and $CsBrF_4$ in MeCN. White cryst. Phase change at 80°; dec. at 257°.

Edwards, A.J. *et al*, *J. Chem. Soc. A*, 1969, 1936 (*cryst struct, K salt*)
Christie, K.O. *et al*, *Inorg. Chem.*, 1970, **9**, 1852 (*ir, raman, synth, NO, Cs salts*)
Surles, T. *et al*, *J. Fluorine Chem.*, 1973, **3**, 293, 453 (*raman*)
Sukhoverkhov, V.F. *et al*, *Zh. Neorg. Khim.*, 1980, **25**, 3041 (*synth, Ag salt*)
Mahjoub, A.R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 1526 (*synth*)
Wilson, W.W. *et al*, *Inorg. Chem.*, 1989, **28**, 4172 (*synth, ir, F-19 nmr, Me_4N salt*)
Christie, K.O. *et al*, *J. Fluorine Chem.*, 1989, **43**, 125 (*synth*)

$BrF_4^{\oplus}$ IC-001658

Tetrafluorobromine(1+)
[41646-52-0]



M 155.8 (ion)
Br—F 177, 185 pm. Colourless cation. Reacts violently with H_2O.
Hexafluoroantimonate:
$BrF_{10}Sb$ M 391.6
Synth. from stoichiometric quantities of BrF_5 and SbF_5.
μ-Fluorodecafluorodiantimonate: [36445-03-1].
$BrF_{15}Sb_2$ M 608.3
Synth. from $2SbF_5$ and BrF_5 at 120°. Used to extract Xe and Rn from the atm. White cryst.

Meinert, H. *et al*, *Z. Chem.*, 1970, **10**, 226 (*ir, F-19 nmr, $Sb_2F_{11}^{\ominus}$*)
Lind, M.D. *et al*, *Inorg. Chem.*, 1972, **11**, 608 (*cryst struct, $Sb_2F_{11}^{\ominus}$*)
Surles, T. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 3561 (*raman, synth, $Sb_2F_{11}^{\ominus}$*)
Kuz'min, A.I. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2127; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1178 (*struct, nqr*)
Baran, E.J., *J. Fluorine Chem.*, 1981, **17**, 543 (*ir, raman*)

BrF_4Mo IC-001659

Molybdenum bromide fluoride ($MoBrF_4$), 9CI
[25081-79-2]

$MoBrF_4$

M 251.8
Prob. has a polymeric struct. Prepd. from MoF_6 and $MoBr_4$. Non-volatile red-brown, glassy solid.

Mercer, M. *et al*, *J. Chem. Soc. A*, 1969, 2532 (*synth*)

BrF_5 IC-001660

Bromine fluoride (BrF_5)
Bromine pentafluoride
[7789-30-2]

BrF_5

M 174.8
Square based pyramid with Br sl. below the square base. Base bond length 178 pm, apex bond length 168 pm. Base/apex angle 84.5°. Commercially available. Colourless liq. Extremely vigorous fluorinating agent. d^{25} 2.466. Mp −60.5°. Bp 40.5°. ΔH_f° −429 kJ mol^{-1}.
▷ Reacts violently with H_2O. EF9350000.

Burbank, R.D. *et al*, *J. Chem. Phys.*, 1957, **27**, 981 (*cryst struct*)
Muetterties, E.L. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 1084 (*F-19 nmr*)
Stein, L., *J. Am. Chem. Soc.*, 1959, **81**, 1269 (*synth*)
Begun, G.M. *et al*, *J. Chem. Phys.*, 1965, **42**, 2236 (*ir*)
Stein, L., *Halogen Chem.*, (Gutmann, V., Ed.) Academic Press, London, 1967, 168 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 246 (*props*)

BrF_5NRe IC-001661

Rhenium(*VII*) bromoimide pentafluoride
[Bromamidato(2−)]pentafluororhenium(VII), *12CI*
[107605-54-9]

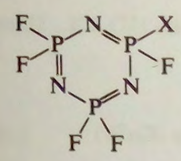
$ReF_5(NBr)$

M 375.1
Synth. from ReF_3N and BrF_3. Deep purple hygroscopic solid. Mp 140°. Subl. 150° *in vacuo*.

Fawcett, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 567 (*synth, ir*)

$BrF_5N_3P_3$ IC-001662

2-Bromo-2,4,4,6,6-pentafluoro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 9CI, 8CI
Bromopentafluorocyclotriphosphonitrile. Bromopentafluorocyclotriphosphazene. 2-Bromo-2,4,4,6,6-pentafluoro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2-Bromo-2,4,4,6,6-pentafluoro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine
[17022-75-2]



X = Br

M 309.8
Synth. from $P_3N_3Br_6$ + AgF. Colourless liq., fumes in moist air. Bp 97°. Selectively reactive to nucleophiles at Br.

Steger, E. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1812 (*synth, gc, ir*)
Glemser, O. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 282 (*synth, ir, F-19 nmr*)
Chivers, T. *et al*, *J. Chem. Soc. A*, 1970, 2324 (*synth, F-19 nmr*)
Roesky, H.W. *et al*, *Z. Naturforsch., B*, 1974, **29**, 174 (*reactions*)

BrF_5OSe IC-001663

Selenium(*VI*) fluoride hypobromite ($SeF_5(OBr)$)
[40217-25-2]

$BrOSeF_5$

M 269.8
Formed from $(F_5SeO)_3Br$ + Br_2. Red liq. Mp −85°. Bp 67°.

Seppelt, K., *Chem. Ber.*, 1972, **106**, 157 (*synth, ir, ms*)

BrF_5S IC-001664

Sulfur(*VI*) bromide fluoride ($SBrF_5$)
Sulfur bromide pentafluoride. Bromopentafluorosulfur
[15607-89-3]

$BrSF_5$ (C_{4v})

M 206.9
Interatomic distances: F—S 159.7, S—Br 219.0 pm. Formed by reaction of S_2F_{10} + Br_2. Colourless gas. Mp −79°. Bp 3.1°. Dec. at 150° to SF_6, SF_4, Br_2.

Neuvar, E.W. *et al*, *J. Chem. Phys.*, 1963, **39**, 596 (*struct*)
Kovacina, T.A. *et al*, *J. Fluorine Chem.*, 1976, **7**, 430 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 9, *Suppl. Vol.*, 1978, B2, 300 (*bibl*)

BrF_5Sn_3 IC-001665

Tin bromide fluoride (Sn_3BrF_5)
Tritin bromide pentafluoride. Bromopentafluorotritin
[12431-51-5]

Sn_3BrF_5

M 531.0
Sn has 3-coord. pyramidal struct. Solid struct. built up of $(Sn_{12}F_{20})_n^{4n\oplus}$ macrocations which interconnect to form infinite layers. Synth. from SnF_2 and $SnBr_2$. Colourless rod shaped cryst.

Donaldson, J.D. *et al*, *J. Chem. Soc. A*, 1969, 2358 (*synth, struct, mössbauer*)
Lari-Lavessani, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **281**, 535 (*synth, cryst struct*)
Vilminot, S. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 35 (*cryst struct*)
Claudy, P. *et al*, *J. Fluorine Chem.*, 1981, **18**, 203 (*cryst struct*)

$BrF_5Ta^{\ominus}$ IC-001666

Bromopentafluorotantalate(*V*)(1−), 11CI
[35220-71-4]

$[TaBrF_5]^{\ominus}$ (C_{4v})

M 355.8 (ion)
Octahedral anion. A number of mixed halide complexes $[TaX_5Y]^{\ominus}$ are formed in the same way.
H compd.: [98538-90-0].
BrF_5HTa M 356.8
Synth. as the $(Et_2O)_2H$ salt by dissolving TaF_5 in Et_2O saturated with HBr. Light yellow hygroscopic solid + $2Et_2O$. Sol. DMF; sl. sol. MeCN, Me_2CO, alcohols. Adducts with Py or ethylenediamine are also formed.

Buslaev, Yu.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1971, **20**, 99; *CA*, **76**, 52623u (*nmr*)
Papadimitriou, C. *et al*, *J. Less-Common Met.*, 1985, **108**, 217 (*synth, ir*)

IC-001667

BrF_4Te

Tellurium(*VI*) bromide fluoride ($TeBrF_5$)

Tellurium bromide pentafluoride. Bromopentafluorotellurium

[21975-45-1]

$BrTeF_5$ (C_{4v})

M 302.4

Synth. from TeF_4 + Br_2. Red liq., stable at −78°.

Lawlor, L. *et al, Inorg. Chem.*, 1979, **18**, 2921 (*synth, ir, raman, F-19 nmr*)

Lawlor, L., *Diss. Abstr. Int., B*, 1981, **42**, 2362 (*synth, ir, raman*)

IC-001668

$BrF_4^{\ominus}$

Hexafluorobromate(*V*)(1−)

[56713-48-5]

$[BrF_6]^{\ominus}$ (O_h)

M 193.8 (ion)

▷ Reacts explosively with H_2O.

Cs salt: [26222-92-4].

$BrCsF_6$ M 326.8

Colourless cryst. Dec. on heating. Representative of the alkali metal salts.

Me_4N salt: [35064-02-9].

Hazardous synth. from $[Me_4N]F$ and $CsBrF_6$ in MeCN. White cryst. (slowly dec. at r.t., possibly to BrF_4 salt). Dec. at 220°.

Bougon, R. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1971, **272**, 565 (*ir, raman*)

Meinert, H. *et al, Z. Chem.*, 1971, **11**, 469 (*raman, synth, salts*)

Mahjoub, A.R. *et al, Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 1526 (*synth*)

Christie, K.O. *et al, Inorg. Chem.*, 1989, **28**, 3275 (*synth, F-19 nmr, Cs salt, raman*)

Wilson, W.W. *et al, Inorg. Chem.*, 1989, **28**, 4172 (*synth, ir, Me_4N salt*)

IC-001669

$BrF_4^{\oplus}$

Hexafluorobromine(I+)

[51063-27-5]

$[BrF_4]^{\oplus}$

M 193.8 (ion)

Octahedral, Br—F 169 pm. Colourless ion, powerful fluorinating agent. Readily oxidises O_2 and Xe (g).

▷ Reacts violently with H_2O.

Hexafluoroarsenate: [51063-29-7].

$AsBrF_{12}$ M 382.8

Synth. from BrF_3 and $[KrF]AsF_6$ in BrF_3. White solid.

Hexafluoroantimonate: [53432-26-1].

$BrF_{10}Sb$ M 429.6

Synth. from $BrF_4[Sb_2F_{11}]$ in BrF_3 and KrF_2. White solid + < 1 SbF_5.

μ-Fluorodecafluorodiantimonate: [51063-28-6].

$BrF_{17}Sb_2$ M 646.3

Synth. from BrF_3 and $[Kr_2F_3][SbF_6]$ in BrF_3. White solid.

[52707-24-1]

Gillespie, R.J. *et al, Inorg. Chem.*, 1974, **13**, 1230 (*synth, F-19 nmr, raman*)

Christie, K.O. *et al, Inorg. Chem.*, 1975, **14**, 694 (*struct, synth, ir*)

Baran, E.J. *et al, Indian J. Pure Appl. Phys.*, 1982, **20**, 152.

IC-001670

BrF_5NS

Sulfur(*VI*) bromofluoroamide fluoride ($S(NBrF)F_4$)

Sulfur bromofluoramide pentafluoride. (Bromafluoramido) pentafluorosulfur, 11CI

[90388-94-6]

$BrN(F)SF_5$

M 239.9

Synth. from $F_4S{=}NF$ + Br_2 + KF. Pale green liq., mod. stable at 20°.

O'Brien, B.A. *et al, Inorg. Chem.*, 1984, **23**, 2188 (*synth, F-19 nmr*)

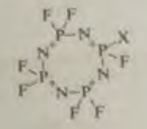
IC-001671

$BrF_7N_4P_4$

2-Bromo-2,4,4,6,6,8,8-heptafluoro-2,2,4,4,6,6,8,8-octahydro-1,3,5,7,2,4,6,8-tetrazatetraphosphocine, 8CI

Bromoheptafluorocyclotetraphosphanitrile. Bromoheptafluorocyclotetraphosphazene. 2-Bromo-2,4,4,6,6,8,8-heptafluoro-2λ⁵,4λ⁵,6λ⁵,8λ⁵-cyclotetraphosphaza-1,3,5,7-tetraene

[23208-37-9]



X = Br

M 392.8

Synth. by reaction of $P_4N_4F_7(NMe_2)$ + HBr. Liq. Bp 134°.

Chivers, T. *et al, J. Chem. Soc. A*, 1970, 2324 (*synth, F-19 nmr*)

IC-001672

$BrF_{15}O_5Se_3$

Tris(pentafluorooxyselenato)bromine

Bromine(III) pentafluorooxyselenate

[39989-16-7]

$Br(OSeF_5)_3$

M 649.7

Formed from BrF_3 + $HOSeF_5$. Yellow viscous liq. Mp 19° $Bp_{0.2}$ 43°.

Seppelt, K., *Chem. Ber.*, 1973, **106**, 157, 1920 (*synth, F-19 nmr, ir, ms*)

IC-001673

BrGa

Gallium(*I*) bromide (GaBr)

[22655-59-0]

GaBr

M 149.6

Known as gas-phase sp. Synth. from Ga + $GaBr_3$ or generated in electrothermal carbon furnace. Important sp. in chemical vapour transport of GaAs. ΔH_f° −17.6 kJ mol^{-1}; S° 251.5 J K^{-1} mol^{-1}.

Faktor, M.M. *et al, J. Chem. Soc., Faraday Trans. 1*, 1977, **73**, 1446 (*thermodyn props, use*)

Pfaffe, S. *et al, Z. Naturforsch., A*, 1978, **33**, 1386 (*microwave*)

Tsunoda, K. *et al, Spectrochim. Acta, Part B*, 1980, **35**, 715 (*ir, use*)

Rajappan Naiv, K.P. *et al, Chem. Phys. Lett.*, 1981, **80**, 149 (*microwave*)

IC-001674

BrGaO

Gallium bromide oxide (GaBrO)

Gallium(III) oxide bromide

GaBrO

M 165.6

Synth. from Ga_2O_3 and $GaBr_3$ at 230-250°. White solid. Mod. sol. H_2O; insol. alcohols, ethers, hydrocarbons. Mp 230° dec.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1963, **321**, 85 (*synth, props, powder struct*)

Brewer, F.M. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 361 (*synth, props*)

IC-001675

BrGaS

Gallium(*III*) bromide sulfide (GaBrS)

GaBrS

M 181.6

Synth. from $GaBr_3$, Ga and S at 305-345°. Colourless moisture-sensitive cryst. Mp 360° dec.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1963, **321**, 85 (*synth, props, powder struct*)

IC-001676

BrGaSe

Gallium(*III*) bromide selenide (GaBrSe)

GaBrSe

M 228.5

Synth. from $GaBr_3$, Ga and Se at 300-340°. Colourless moisture-sensitive needles. Mp 280° dec.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1963, **321**, 85 (*synth, props, powder struct*)

IC-001677

BrGaTe

Gallium(*III*) bromide telluride (GaBrTe)

GaBrTe

M 277.2

Synth. from $GaBr_3$, Ga and Te at 260-270°. Yellow moisture-sensitive needles. Mp 250° dec. Related compd. Ga_3Te_3Br also descr.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1963, **321**, 85 (*synth, props, powder struct*)

Paashaus, S. *et al, Angew. Chem., Int. Ed. Engl.*, 1986, **25**, 752 (*related compd*)

IC-001678

$BrGeH_3$

Bromogermane, 9CI

[13569-43-2]

GeH_3Br

M 155.5

Synth. by direct reaction of Br_2 with GeH_4. Liq. $d_4^{29.5}$ 2.34. Mp −32°. Bp 52°.

Cradock, S. *et al, J. Mol. Struct.*, 1981, **74**, 265 (*struct*)

Inorg. Synth., 1974, **15**, 157 (*synth*)

Anderson, J.W. *et al, Can. J. Chem.*, 1972, **50**, 1607 (*synth*)

Mackay, K.M. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 1377 (*synth*)

Ebsworth, E.A.V. *et al, J. Mol. Spectrosc.*, 1964, **12**, 299 (*pmr*)

Griffiths, J.E. *et al, Can. J. Chem.*, 1962, **40**, 579 (*ir*)

Freeman, D.E. *et al, J. Chem. Phys.*, 1963, **39**, 2908 (*ir*)

Dennis, L.M. *et al, J. Am. Chem. Soc.*, 1929, **51**, 2321 (*synth*)

Buerger, H. *et al, J. Mol. Spectrosc.*, 1983, **97**, 266 (*ir*)

IC-001679

BrH

Hydrogen bromide

Hydrobromic acid, 9CI

[10035-10-6]

HBr

M 80.9

H—Br 141.4 pm. Prepd. by catalytic combination of H_2 and Br_2, from the action of H_2SO_4 on KBr, or from tetrahydronaphthalene and Br_2. Formed as a by-product in the bromination of org. compds. Commercially available. A brominating and reducing agent in org. and inorg. synth. Colourless, nonflammable gas with an acrid odour. Fumes strongly in moist air. Aq. solns. are strongly acid. V. sol. H_2O. Sol. EtOH. Mp −87°. Bp −66.5°. ΔH_f° −36.4 kJ mol^{-1}; ΔG_f° −53.45 kJ mol^{-1}; S_f° 198.59 J K^{-1} mol^{-1}; Ir ν_{H-Br} 2650 cm^{-1}.

▷ Mildly toxic by inhalation. Irritant to eyes and skin. MW3850000.

Dihydrate: [13465-04-8].
Mp −11.3°.

Trihydrate: [30981-42-1].
Mp −47.9°.

Tetrahydrate: [22822-60-2].
Mp −55.8°.

Inorg. Synth., 1939, **1**, 149 (*synth*)

Savoie, R. *et al, J. Chem. Phys.*, 1966, **44**, 548 (*ir, raman*)

Lundgren, J.O. *et al, J. Chem. Phys.*, 1968, **49**, 1068 (*cryst struct, tetrahydrate*)

Lundgren, J.O. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 1893 (*cryst struct, hydrates*)

Gilbert, A.S. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 337 (*ir, hydrates*)

Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1280 (*rev*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 296 (*synth*)

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 244 (*rev*)

Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1900.

IC-001680

$BrHHgO_4$

Mercury bromate hydroxide ($HgBrO_3(OH)$)

[11092-91-4]

$Hg(OH)BrO_3$

M 345.4

Struct. comprises near planar infinite zig-zag chains of $[-(OH)-Hg-(OH)-]_n^{n\oplus}$ and separate $BrO_3^{\ominus}$ linked by H-bonding. Obt. from $KBrO_3$ and hot 0.2*M* $Hg(NO_3)_2$ soln. Cryst. (H_2O). Sl. sol. H_2O (81 mg per 100 ml at 25°).

Smith, G.F., *J. Am. Chem. Soc.*, 1924, **46**, 1577 (*synth*)

Weiss, A. *et al, Z. Naturforsch., B*, 1960, **15**, 678 (*cryst struct*)

Bjornlund, G., *Acta Chem. Scand.*, 1971, **25**, 1645 (*synth, cryst struct*)

IC-001681

BrHO

Hypobromous acid, 11CI

[13517-11-8]

HOBr

M 96.9

Salts slowly disproportionate to $Br^{\ominus}$ and $BrO_3^{\ominus}$, catalysed by $Br^{\ominus}$. Synth. from Br_2 + H_2O + $AgNO_3$ (HgO). Strong bleaching agent. Strong oxidant, exists at 20° only in aq. soln. (< 7% HOBr). pK_a 8.8.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1922, **2**, 243; *Part* 1, 1956, **2/II**, 750 (*synth, props*)
Radford, P.J.M., *Bromine and its Compounds*, Jolles, Z.E., Ed., 1966, 154 (*synth, props*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 320, 321 (*synth, Na, K salts*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 247.

$BrHO_2$ IC-001682

Bromous acid, 11CI

[37691-27-3]

HOBr=O

M 112.9

Synth. by reaction of $Br_2 + H_2O + AgNO_3$. Commercially available as the ion in $NaBrO_2.3H_2O$. Used to remove starches from fabrics. Sol. H_2O.

Na salt: see *Sodium bromite*, *IC-001730*

Richards, A.H., *J. Soc. Chem. Ind., London*, 1906, **25**, 4 (*synth*)
Sourisseau, G., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1948, **226**, 1605.
Radford, P.J.M., *Bromine and its Compounds*, Jolles, Z.E., Ed., 1966, 159 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 248.

$BrHO_2Se$ IC-001683

Bromoselenious acid

[88212-41-3]

O=Se(Br)OH

M 191.8

Present in solns. of SeO_2 in HBr.

Futekov, L. *et al, Z. Anal. Chem*, 1975, **276**, 41 (*raman*)
Milne, J. *et al, Inorg. Chem.*, 1985, **24**, 840 (*formn, equilibria in soln, raman*)

$BrHO_3$ IC-001684

Bromic acid

[7789-31-3]

$HOBrO_2$

M 128.9

Stable as salts. Formed as the anion by electrolysis of $Br^{\ominus}$ solns. Strong oxidising agent. Aq. solns. stable up to 50% at 40°. Dec. to $Br_2 + O_2 + H_2O$. Sol. H_2O. pK_a 0.7.

Na salt: see *Sodium bromate(V)*, *IC-001731*
K salt: see *Potassium bromate(V)* ($KBrO_3$), *IC-001712*

Ewing, D.T. *et al, Trans. Electrochem. Soc.*, 1925, **47**, 117 (*synth*)
Bogatyrev, V.I. *et al, J. Appl. Chem. USSR (Engl. Transl.)*, 1963, **36**, 205 (*synth*)
Brauer, G., *Handbuch Prdp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 325 (*synth, Ba salt*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 248.

$BrHO_4$ IC-001685

Perbromic acid

[19445-25-1]

$HOBrO_3$

M 144.9

Strong monobasic acid. Synth. by oxidation of $BrO_3^{\ominus}$ with F_2 in alk. soln. Strong oxidant. Stable to 6*M* (55%) aq. soln. at 100°.

K salt: see *Potassium perbromate* ($KBrO_4$), *IC-001713*
Rb salt: see *Rubidium perbromate* ($RbBrO_4$), *IC-001747*

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1922, **2**, 384; *Part* 1, 1956, **2/II**, 770 (*rev*)
Johnson, G.K. *et al, Inorg. Chem.*, 1970, **9**, 119 (*thermodynamics, props*)
Inorg. Synth., 1972, **13**, 1 (*synth, props*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 331, 333 (*synth, K salt, NH_4 salt*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 249.

BrHZr IC-001686

Zirconium bromide hydride (ZrBrH), 11CI

[60921-40-6]

HZrBr

M 172.1

Hydrides occupy the tetrahedral sites between the metal layers of the ZrBr structure which contains the layer sequence Br—Zr—Zr—Br. Synth. by heating ZrBr in H_2 for several days at 300°. Bronze solid.

Deutero compd.: [97055-83-9]. *Zirconium bromide deuteride*
BrDZr M 173.1
Bronze solid. Pairs of deuterides are located 25pm inside opposite trigonal faces of O_h holes in the Zr layers of the ZrBr struct.

Murphy, P.D. *et al, J. Chem. Phys.*, 1979, **70**, 4552 (*nmr*)
Corbett, J.D. *et al, Inorg. Chem.*, 1983, **22**, 3194 (*pe*)
Marek, H.S. *et al, J. Less-Common Met.*, 1983, **89**, 243 (*synth, cryst struct*)
Wijeyesekera, S.D. *et al, Solid State Commun.*, 1985, **54**, 657 (*deuteride, nd, struct, synth*)

BrH_2N IC-001687

Bromamide, 11CI, 10CI, 9CI

Monobromamine

[14519-10-9]

$BrNH_2$

M 95.9

Synth. from $NH_3 + Br_2$ at −60°. Violet-black solid. Sol. Et_2O, insol. pentane. pK_a 6.39.

▷ Dec. violently above −70° when pure.

Coleman, G.H. *et al, J. Am. Chem. Soc.*, 1934, **56**, 965 (*synth*)
Jander, J. *et al, Z. Anorg. Allg. Chem.*, 1967, **349**, 57 (*synth, props*)
Clemens, D.F. *et al, Inorg. Chem.*, 1969, **8**, 998 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 243.
Soulard, M. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 2300 (*anal, equilibria in soln*)
Greene, D.J., *Water Eng. Manag.*, 1981, **128**, 47 (*use*)

$BrH_3Mn_2O_3$ IC-001688

Manganese(*II*) bromide hydroxide ($Mn_2Br(OH)_3$)

Bromotrihydroxodimanganese(II)

$Mn_2(OH)_3Br$

M 240.8

Synth. from boiling 1.5*M* aq. $MnBr_2$ and Mn powder in absence of air. Cryst. Rhombic struct.

Oswald, H.R. *et al, Helv. Chim. Acta*, 1964, **47**, 272 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, **C5**, 308 (*rev, bibl*)

BrH_3Si IC-001689

Bromosilane

SiH_3Br

M 111.0

Colourless gas at r.t. d^{-80} 1.72, d^0 1.533. Mp −94°. Bp 1.9°.

▷ Explodes in air.

Arnold, D.E.J. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2518 (*synth, nmr*)
Voronkov, M.G. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **232**, 817 (*ir*)
Olah, G.A. *et al, Organometallics*, 1982, **1**, 1485 (*Si-29 nmr*)

BrH_3Sn IC-001690

Bromostannane

[32013-93-7]

$SnBrH_3$ (C_{3v})

M 201.6

Unstable, lifetime 10-30 mins. at 0° and <10m bar.

Wolf, S.N. *et al, J. Chem. Phys.*, 1971, **54**, 4605 (*synth, microwave*)
Buerger, H. *et al, Z. Naturforsch., A*, 1985, **40**, 989 (*ir*)
Betzel, M. *et al, Z. Naturforsch., A*, 1986, **41**, 1009 (*ir*)

BrH_4N IC-001691

Ammonium bromide

[12124-97-9]

$[NH_4]^{\oplus}Br^{\ominus}$ (cubic)

M 97.9

Synth. from $NH_3 + Br_2$ or from NH_3 + HBr. Commercially available. Has pharmaceutical and photographic applications. White cryst. solid, subl. when heated. V. sol. H_2O. d_4^{20} 2.40. Subl. 400°. V.p. 862 mm at 400°.

▷ BO9170000.

Tetra-deutero compd.: [12265-06-4]. *Tetradeuteroammonium bromide*
BrD_4N M 101.9
Synth. from NH_4Br + excess D_2O. Commercially available. Tetragonal or cubic cryst. V. sol. H_2O. Interatomic distance: N—D 103 pm.

Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 203.
Levy, H.A. *et al, J. Am. Chem. Soc.*, 1953, **75**, 1536 (*deriv, synth, struct*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, *Part* 1, 1964, **8/I**, 435 (*rev*)
Press, W. *et al, Phys. Rev. B*, 1976, **14**, 1983 (*deriv, nd*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 524.

BrH_4P IC-001692

Phosphonium bromide, 8CI

[24567-52-0]

$PH_4^{\oplus}Br^{\ominus}$

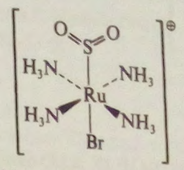
M 114.9

Interatomic distance: P—H 141.4 pm; angle: HPH 108.7°, 109.9°. Synth. from PH_3 + HBr. Gas at r.t.; Rather unstable solid at low temps. Dissociation pressure at 25° ca. 760 mm.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 504 (*bibl*)
Tsang, T. *et al, J. Chem. Phys.*, 1968, **49**, 4403 (*synth, pmr*)
Rush, J.J. *et al, J. Chem. Phys.*, 1969, **51**, 2947 (*raman*)
Durig, J.R. *et al, J. Chem. Phys.*, 1969, **51**, 4449 (*synth, ir, raman*)
Schroeder, L.W. *et al, J. Chem. Phys.*, 1971, **54**, 1968 (*cryst struct*)

$BrH_{12}N_4O_2RuS^{\oplus}$ IC-001693

Tetraamminebromo(sulfur dioxide-*S*)ruthenium(*II*)(1+)



trans-S-bonded form

M 313.1 (ion)

Prepd. by dissolving Tetraamminebis(hydrogen sulfito-*O*) ruthenium(*II*), IC-019924 in boiling aq. HBr. Hydrol. in H_2O → Tetraammine(aqua)(sulfur dioxide-*S*) ruthenium(*II*)(2+), IC-019920.

Bromide:
$Br_2H_{12}N_4O_2RuS$ M 393.0
Brown cryst.

Gleu, K. *et al, Z. Anorg. Allg. Chem.*, 1936, **227**, 237; 1938, **235**, 201, 211 (*synth*)
Vogt, L.H. *et al, Inorg. Chem.*, 1965, **4**, 1157 (*synth, ir, powder struct*)

$BrH_{12}N_5ORu^{2\oplus}$ IC-001694

Tetraamminebromo(nitrosyl)ruthenium(2+), 9CI

$[Ru(NO)Br(NH_3)_4]^{2\oplus}$

M 279.1 (ion)

pseudo-Octahedral cation. Sol. H_2O. A slow *cis* → *trans* isomerisation occurs in basic soln., but is inhibited by acid or in the solid state. Various isotopomers (D, ^{15}N) also known.

***cis*-form**

Dibromide: [38402-58-3].
Synth. by treating *cis*-$[Ru(NH_3)_4Br_2]Br$ with NO in dil. aq. HBr. Orange solid. First prepd. in 1973. Ir ν_{NO} 1934, 1902 cm^{-1}.

***trans*-form** [16482-04-5]

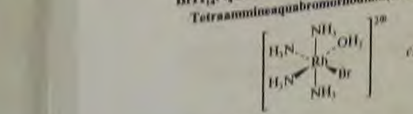
Dibromide: [36400-25-6].
Prepd. by treating *trans*- Tetraammine(hydroxy) (nitrosyl)ruthenium(2+), IC-019914 with conc. HBr, or by thermolysis of $[Ru(NO)(NH_3)_5]Br_3$, or by treating *trans*-$[Ru(NH_3)_4Br_2]Br$ with NO. Known since 1890. Orange salt. Ir ν_{NO} 1891; ν_{Ru-Br} 222 cm^{-1}.

[20956-33-6]

Joly, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1890, **111**, 969 (*synth, trans-form*)
Fairey, M.B. *et al, Spectrochim. Acta*, 1966, **22**, 359 (*ir*)
Armor, J.N. *et al, J. Am. Chem. Soc.*, 1968, **90**, 5928 (*synth, trans-form*)
Schreiner, A.F. *et al, Inorg. Chem.*, 1972, **11**, 880 (*synth, trans-form, uv, mcd*)
Pell, S. *et al, Inorg. Chem.*, 1973, **12**, 873 (*synth, cis and trans-forms, ir, uv*)
Sinitsyn, N.M. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 918 (*stability const*)
Sinitsyn, N.M. *et al, Koord. Khim.*, 1976, **2**, 1381 (*synth, trans-form*)
Sizova, O.V. *et al, Soc. J. Coord. Chem. (Engl. Transl.)*, 1976, **2**, 853 (*theory, uv*)

$BrH_{12}N_4ORh^{2\oplus}$ IC-001695

Tetraamminesquabromorhodium(*III*)(2+), 1OCl



cis-form

M 268.9 (ion)
Octahedral cation.

cis-form [71382-14-4]

Dithionate: [71382-16-6].
Synth. from *cis*-$[Rh(NH_3)_4Br_2]Br·\frac{1}{2}H_2O$, Ag_2O and $Na_2S_2O_4$. Light orange prisms.

trans-form [71424-39-0]

Dithionate: [71424-41-4].
Analogous synth. to *cis*-form using *trans*-$[Rh(NH_3)_4Br_2]Br·\frac{1}{2}H_2O$. Transparent red-brown prisms. Sol. H_2O.

Skibsted, L.H. *et al, Inorg. Chem.*, 1979, **18**, 3171 (*synth, uv, photochem*)

$BrH_{15}N_5Os^{2\oplus}$ IC-001696

Pentaamminebromoosmium(*III*)(2+)

[43031-58-9]

$[OsBr(NH_3)_5]^{2\oplus}$

M 355.2 (ion)
Dibromide: Osmium(III) *bromide pentaammine*
Synth. from $[Os(NH_3)_5(N_2)](ClO_4)_2$ and $H_3Ce(ClO_4)_6$ followed by addition of conc. HBr. λ_{max} 314 nm (ε 1870).

Allen, A.D. *et al, Can. J. Chem.*, 1973, **51**, 92 (*ir*)
Verdonek, E. *et al, Inorg. Chem.*, 1974, **13**, 762 (*uv*)
Bee, M.W. *et al, Spectrochim. Acta, Part A*, 1974, **30**, 139 (*ir*)
Sakaki, S. *et al, J. Phys. Chem.*, 1978, **82**, 1917 (*esr*)
Buhr, J.D. *et al, Inorg. Chem.*, 1980, **19**, 2416 (*synth, uv*)
Lay, P.A. *et al, Inorg. Chem.*, 1989, **28**, 3001 (*uv, ir, electrochem*)

$BrH_{15}N_5Ru^{\oplus}$ IC-001697

Pentaamminebromoruthenium(*II*)(1+), 9Cl

[63284-61-7]

$[Ru(NH_3)_5Br]^{\oplus}$

M 266.1 (ion)
Pseudo-octahedral; undergoes rapid aquation. Prepd. by the chemical or electrochemical reduction of Pentaamminebromoruthenium(*III*)(2+), IC-001698. No salts have been isol. Sol. H_2O.

Lim, H.S. *et al, Inorg. Chem.*, 1972, **11**, 1460 (*synth, electrochem*)
Coleman, G.N. *et al, Inorg. Chem.*, 1973, **12**, 1036 (*synth, kinetics*)

$BrH_{15}N_5Ru^{2\oplus}$ IC-001698

Pentaamminebromoruthenium(*III*)(2+), 10Cl

[21388-15-8]

$[Ru(NH_3)_5Br]^{2\oplus}$ (C_{4v})

M 266.1 (ion)
Reagent for the study of the mechanism of electron-transfer reactions. Readily undergoes aquation and anation reactions; more easily reduced than its chloro analogue.

Dibromide: [16446-65-4]. *Pentaamminebromoruthenium*(III) *bromide. Ruthenium*(III) *bromide pentaammoniate*
$Br_3H_{15}N_5Ru$ M 425.9

Prepd. by heating $[Ru(NH_3)_6]^{3\oplus}$ or $[Ru(NH_3)_5(OH)]^{2\oplus}$ with aq. HBr. Orange-red cryst. (aq. HBr). Less sol. H_2O than $[Ru(NH_3)_5Cl]Cl_2$. Ir ν_{Ru-Br} 210 cm^{-1}. Dec. on heating → $[Ru(NH_3)_3Br_3] + 2NH_3$.

Allen, A.D. *et al, Can. J. Chem.*, 1967, **45**, 1337 (*synth, ir*)
Broomhead, J.A. *et al, Inorg. Chem.*, 1968, **7**, 2519; 1969, **8**, 2124 (*hydrol.*)
Inorg. Synth., 1970, **12**, 2 (*synth*)
Shinohara, T. *et al, Bull. Chem. Soc. Jpn.*, 1972, **45**, 3081 (*anation*)
Lim, H.S. *et al, Inorg. Chem.*, 1972, **11**, 1460 (*electrochem*)
Faraggi, M. *et al, Inorg. Chem.*, 1973, **12**, 236 (*uv, reactions*)
Ohyoshi, A. *et al, Bull. Chem. Soc. Jpn.*, 1974, **47**, 841 (*rga, dta*)
Bee, M.W. *et al, Spectrochim. Acta, Part A*, 1974, **30**, 139 (*ir, raman*)
Evans, R.S. *et al, Inorg. Chem.*, 1975, **14**, 1705 (*mcd*)
Cohen, H. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1056 (*reactions*)
Kobata, S. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 768 (*theory*)
Sakaki, S. *et al, J. Phys. Chem.*, 1978, **82**, 1917 (*esr*)

BrHf IC-001699

Hafnium bromide (HfBr), 11Cl

[49681-62-1]

HfBr

M 258.3
Layer struct. Synth. by heating $HfBr_4$ and Hf at 480-580° and 30-40 atm. Black, graphite-like solid.

Marek, G.S. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 890 (*synth, struct*)

BrHgI IC-001700

Mercury bromide iodide (HgBrI)

[13444-76-3]

HgBrI

M 407.3
Exists in soln. in equilibrium with $HgBr_2$ and HgI_2. Synth. from $HgBr_2$ and HgI_2. Bright yellow phototropic cryst.; melts to orange liq. Insol. H_2O, org. solvs., cold acids.

Eliezer, I., *J. Phys. Chem.*, 1964, **68**, 2722 (*equil const*)
Bateanov, S.S. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1965, 199 (*synth, powder struct, thermal anal*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1967, **B2**, 946 (*rev, bibl*)
Rastogi, R.P. *et al, J. Am. Chem. Soc.*, 1967, **89**, 200 (*synth*)
Clarke, J.H.R. *et al, J. Chem. Phys.*, 1968, **48**, 528 (*raman, molten salt*)
Zangen, M., *J. Inorg. Nucl. Chem.*, 1969, **31**, 869 (*synth*)
Rastogi, R.P. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 1530 (*powder struct*)
Beattie, I.R. *et al, J. Chem. Soc. A*, 1970, 2433 (*raman, vapour*)
Kennard, C.H.L., *J. Inorg. Nucl. Chem.*, 1970, **32**, 2440 (*struct*)
Mal'tsev, A.A. *et al, Nature (London)*, 1971, **231**, 157 (*ir, vapour*)
Givan, A. *et al, J. Chem. Phys.*, 1975, **64**, 1967; 1976, **65**, 1851 (*raman, ir*)
Griffiths, T.R. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 205, 209 (*uv, props*)
Belevantsev, V.I. *et al, Koord. Khim.*, 1980, **6**, 1000 (*uv-vis*)

$BrHg_2P_3$ IC-001701

Mercury bromide phosphide (Hg_2BrP_3)

[39317-05-0]

Hg_2BrP_3

M 574.0
Synth. from $HgBr_2$, Hg and P under pressure and at 500°. Semiconductor. Black cryst. Insol. strong acids. Dec. at 400°.

Donohue, P.C., *J. Solid State Chem.*, 1973, **6**, 587 (*synth, powder struct*)

BrI IC-001702

Iodine bromide (IBr)

Iodine monobromide

[7789-33-5]

IBr

M 206.8
I—Br 248.5 pm. Dark red solid. d_4^{0} 4.414. Mp 41°. Bp 116° dec. ΔH_f° = 10.5 kJ mol^{-1}. Ir ν 269 cm^{-1}.

Meerum-Terwogt, P.C.E., *Z. Anorg. Allg. Chem.*, 1905, **47**, 209 (*synth, dissoc*)
Cole, L.G. *et al, J. Chem. Phys.*, 1952, **20**, 1343 (*dissoc, synth*)
Wakob, M. *et al, Physica B+C (Amsterdam)*, 1986, **139**, 523 (*raman*)
Yewha, A.J. *et al, J. Phys. Chem.*, 1988, **92**, 5523 (*uv*)
Suzuki, M. *et al, J. Mol. Spectrosc.*, 1989, **133**, 233 (*ir, uv*)

$BrI_3^{\ominus}$ IC-001703

Bromodoiodate(*I*)(1−)

[14791-50-5]

$[Br—I—I]^{\ominus}$

M 333.7 (ion)
I—I 278; I—Br 291 pm; angle BrII 178°. Forms dark red salts. Dissociates in H_2O.

Cs salt: [15801-94-2].
Synth. from CsBr and I_2 in H_2O at 25°. Dark cherry-red cryst. Mp 71° dec.

Me_4N salt: [50725-69-4].
Synth. from Me_4NBr and I_2 in hot EtOH. Dark red cryst. Mp 143°.

[102649-02-5]

Inorg. Synth., 1957, **5**, 167 (*synth*)
Carpenter, G.B., *Acta Crystallogr.*, 1966, **20**, 330.
Maki, A.G. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 867 (*ir, raman*)
Guidelli, R. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 1373 (*formn const*)
Parrett, E.W. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 2458 (*synth, ir, raman*)

$BrI_4^{\ominus}$ IC-001704

Bromotetraiodate(1−)

Tetraiodobromide

$[I_2—Br—I_2]^{\ominus}$

M 587.5 (ion)
Bent struct. postulated.

Me_4N salt: [102073-76-7].
Synth. from $[Me_4N]Br$ and I_2 in boiling EtOH. Brilliant metallic green rhombic plates. Mp 124.5°.

Chattaway, F.D. *et al, J. Chem. Soc.*, 1923, **123**, 654 (*synth, Me_4N salt*)
Nour, E.M. *et al, J. Phys. Chem.*, 1986, **90**, 2841 (*ir, raman*)

$BrI_6^{\ominus}$ IC-001705

Hexaiodobromate

Bromohexaiodate

Struct. unknown

M 841.3 (ion)

Me_4N salt: Synth. from $[Me_4N]BrI_4$ and I_2 in I_2 saturated boiling EtOH. Metallic dark green plates. Mp 109°.

Chattaway, F.D., *J. Chem. Soc.*, 1923, **123**, 654 (*synth*)

BrIn IC-001706

Indium(*I*) bromide (InBr)

[14280-53-6]

InBr

M 194.7
Has yellow TlI struct. with 5-coord. (square pyramidal) In. Synth. from In + $HgBr_2$ at 350°. Red solid. Mp 285°.

Stephenson, N.C. *et al, Aust. J. Sci. Res., Ser. A*, 1950, 580 (*cryst struct*)
Morawietz, W. *et al, Z. Anorg. Allg. Chem.*, 1962, **316**, 220 (*synth*)
Inorg. Synth., 1963, **7**, 18 (*synth*)
Goggin, P.L. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 2501 (*synth, complexes*)
Davies, J.E. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 805 (*raman*)
Tiemann, E. *et al, Z. Naturforsch., A*, 1977, **32**, 6 (*gas phase, rotation spect*)
Tsunoda, K. *et al, Spectrochim. Acta, Part B*, 1980, **35**, 715 (*uv gas*)

BrInO IC-001707

Indium(*III*) bromide oxide (InBrO)

Indium oxybromide

[13776-77-7]

InOBr

M 210.7
Isomorphous with FeOCl. From $InBr_3$, $In(OH)_3$ and H_2O at 300° in a sealed tube. White needles. Spar. sol. H_2O, EtOH, Et_2O. Dec. in dil. acids.

Forsberg, H.-E., *Acta Chem. Scand.*, 1956, **10**, 1287 (*synth, cryst struct*)
Goggin, P.L. *et al, J. Chem. Soc. A*, 1966, 1004 (*synth, props*)
Batsanov, S.S., *J. Struct. Chem. USSR (Engl. Transl.)*, 1968, **9**, 339 (*rev*)
Svergun, V.I. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1970, 1676 (*nqr*)

BrInS IC-001708

Indium(*III*) bromide sulfide (InBrS)

[75492-08-9]

InBrS

M 226.7
Has $CdCl_2$ struct. Synth. from $InBr_3$ and In_2S_3 at 200-225°. Bright grey cryst. Slow dec. in H_2O. Dec. in acids.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1960, **304**, 100; 1962, **314**, 307 (*synth, props, struct*)

BrInSe IC-001709

Indium(*III*) bromide selenide (InBrSe)

InBrSe

M 273.6
Has $CdCl_2$ struct. Synth. from $InBr_3$ and In_2Se_3 at 380-440°. Brown cryst. Slow dec. in H_2O. Dec. by acids. Mp 690-750°.

Hahn, H. *et al, Z. Anorg. Allg. Chem.*, 1960, **304**, 100; 1962, **314**, 307 (*synth, props, powder struct*)
Kniep, R. *et al, Z. Naturforsch., B*, 1981, **36**, 1520 (*phase diagram*)

BrInTe IC-001710

Indium(III) bromide telluride (InBrTe)

[74403-78-4]

InBrTe

M 322.3
Monoclinic layer struct. has trigonal pyramidal coordn. at Te and In_2Te_2Br tetrahedra which share corners and Te—Te edges. Synth. from $InBr_3$ and In_2Te_3 melt. Yellow brown cryst. Slow dec. by H_2O, dec. by acids. Mp 470-510°. E_g 2.45 eV. Ext. compd. In_2Te_2Br. Mp 381°, also dimer.

Hahn, H. *et al*, *Z. Anorg. Allg. Chem.*, 1960, **304**, 100; 1962, 314, 307 (*synth, propr, struct*)
Krieg, R. *et al*, *Mater. Res. Bull.*, 1980, **15**, 783 (*phase diagram*)
Krieg, R. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1520 (*cryst struct, phase diagram*)
Pfuhlmann, S. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1986, **25**, 752 (*rel compd*)

BrK IC-001711

Potassium bromide (KBr), 8CI

[7758-02-3]

KBr

M 119.0
NaCl struct. Synth. either by action of Br_2 on KOH followed by reduction using HCOOH or by neutralisation of KOH or K_2CO_3 with HBr. Commercially available. Used as cell windows for ir spectroscopy. Used in photographic developers, pharmaceuticals and as a bromination agent in org. synth. Formerly used as a sedative. Sl. hygroscopic colourless cubic cryst. V. sol. H_2O (53 g per 100 cm^3 at 0°; 102 g per 100 cm^3 at 100°); spar. sol. EtOH (0.14 g per 100 cm^3 at 25°). Et_2O. Mp 734°. Bp 1435°. ΔH_f° −393.8 kJ mol^{-1}; ΔG_f° −380.4 kJ mol^{-1}; S° 95.9 J K^{-1} mol^{-1}.

▷ Irritant. TS7650000.

Minnigal, A., *Z. Phys.*, 1934, **88**, 178 (*ir*)
Duncan, J., *Compt. Rend Hebd Seances Acad. Sci.*, 1945, **220**, 196 (*ir*)
de Cagnac, A. *et al*, *Compt. Rend Hebd. Seances Acad. Sci.*, 1964, **258**, 4501 (*cryst struct*)
Bowers, G. *et al*, *Phys. Rev.*, 1968, **165**, 391 (*Br-79 nmr*)
Sahm, W. *et al*, *Z. Naturforsch., A*, 1974, **29**, 1754 (*K-39 nmr*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 433 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2896B (*haz*)

$BrKO_3$ IC-001712

Potassium bromate(V) ($KBrO_3$)

Bromic(V) acid, potassium salt, 8CI

[7758-01-2]

$KBrO_3$

M 167.0
Synth. by neutralisation of K_2CO_3 with aq. $HBrO_3$. Commercially available. Powerful brominating agent for deactivated aromatics in sulfuric acid. Also used as an oxidising agent. Colourless hexagonal cryst. Sol. H_2O (13 g per 100 cm^3 at 40°; 50 g per 100 cm^3 at 100°); spar. sol. EtOH; insol. Me_2CO. Mp 434°. ΔH_f° −360 kJ mol^{-1}; ΔG_f° −271 kJ mol^{-1}; S° 149 J K^{-1} mol^{-1}. Pyroelectric.

▷ Oxidiser, toxic, cancer suspect agent. EF8725000.

Swanson, H.E. *et al*, *Natl. Bur. Std. Circ.*, 1955, **7**, 38 (*cryst struct*)
Stierstl, W. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **383**, 231 (*ir*)
Okado, J. *et al*, *J. Phys. Soc. Jpn.*, 1972, **32**, 1412 (*K-39 nmr*)
Kondilenko, I.I. *et al*, *Opt. Spektrosk.*, 1975, **38**, 689 (*raman*)
Harrison, J.J. *et al*, *J. Org. Chem.*, 1981, **46**, 2169 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2896A (*haz*)

$BrKO_4$ IC-001713

Potassium perbromate ($KBrO_4$)

Potassium bromate(VII). Perbromic acid, potassium salt, 8CI

[22207-96-1]

$KBrO_4$

M 183.0
Isotypic with $BaSO_4$. Synth. by oxidation of $KBrO_3$ with F_2 in alkaline soln. Orthorhombic cryst. Dec. on heating by oxygen loss forming $KBrO_3$. ΔH_f° −288 kJ mol^{-1}; ΔG_f° −175 kJ mol^{-1}; S° 170 J K^{-1} mol^{-1}. Dec. at 280°.

▷ Oxidiser.

Appelman, E.H., *Inorg. Chem.*, 1969, **8**, 223 (*synth, ir, raman*)
Siegel, S. *et al*, *Inorg. Chem.*, 1969, **8**, 1190 (*struct*)
Schreiner, F. *et al*, *Inorg. Chem.*, 1970, **9**, 2320 (*thermodynamics*)
Ustupov, V.K. *et al*, *Zh. Neorg. Khim.*, 1975, **20**, 1492 (*stability*)

BrLaO IC-001714

Lanthanum(III) bromide oxide (LaBrO)

Lanthanum oxybromide

[13875-40-6]

LaOBr

M 234.8
Isostructural with PbClF. Cryst. May be doped with rare earths eg. Ce, Th, Eu. for luminescent screens.

Meyer, I. *et al*, *Inorg. Chem.*, 1965, **4**, 1637 (*cryst struct*)
Bärnighausen, H. *et al*, *Z. Anorg. Allg. Chem.*, 1965, **338**, 250 (*synth, ir*)
Rulmont, A., *Spectrochim. Acta*, 1972, **28**, 1287 (*ir, raman*)
Holisa, J. *et al*, *J. Therm. Anal.*, 1982, **25**, 127 (*tga*)
Häuseler, H., *Spectrochim. Acta, Part A*, 1982, **38**, 507 (*ir, raman*)

BrLi IC-001715

Lithium bromide (LiBr), 8CI

[7550-35-8]

LiBr

M 86.8
NaCl struct. Prepd. by slow neutralisation of Li_2CO_3 with aq. HBr; crystallises as the hydrate. Commercially available. Powerful desiccant used in air conditioning and industrial drying systems. Deliquescent white cubic cryst. V. sol. H_2O (145 g per 100 cm^3 at 4°; 254 g per 100 cm^3 at 90°), EtOH (73 g per 100 cm^3 at 40°); mod. sol. MeOH, EtOH, Me_2CO; spar. sol. Py. Mp 550°. Bp 1265°. ΔH_f° −350.9 kJ mol^{-1}; ΔG_f° −341.6 kJ mol^{-1}; S° 74.1 J K^{-1} mol^{-1}.

▷ OJ5755000.

Monohydrate: [23303-71-1].
BrH_2LiO M 104.8
Commercially available. White orthorhombic cryst.; transforms to cubic polymorph. at 33°; dec. on heating with H_2O loss (−H_2O at 165°). V. sol. H_2O (246 g per 100 cm^3 at 20°); sol. EtOH. ΔH_f° −663 kJ mol^{-1}; ΔG_f° −594 kJ mol^{-1}; S° 110 J K^{-1} mol^{-1}.

Dihydrate: [13453-70-8].

BrH_4LiO_3 M 122.8
Colourless cryst.; dec. on heating with H_2O loss (−H_2O at 160°). V. sol. H_2O (246 g per 100 cm^3 at 20°); sol. EtOH. ΔH_f° −963 kJ mol^{-1}; ΔG_f° −841 kJ mol^{-1}; S° 162 J K^{-1} mol^{-1}.

Sigma-Aldrich Library of Chemical Safety Data, **2**, 2151C, 2151D
Davey, W.P., *Phys. Rev.*, 1923, **21**, 143 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 410, 418 (*rev, bibl, deriv*)
Weiss, E. *et al*, *Chem. Ber.*, 1969, **102**, 632 (*cryst struct, pmr, monohydrate*)
Manowa, M. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **396**, 279 (*thermal dec, hydrates*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 439 (*thermochem data*)

$BrLiO_3$ IC-001716

Lithium bromate(V)

Bromic acid, lithium salt, 8CI

[13550-28-2]

$LiBrO_3$

M 134.8
Prepd. by reaction of aq. $Ba(BrO_3)_2$ with aq. Li_2SO_4. Deliquescent colourless orthorhombic cryst. Sol. H_2O. Mp 260°. ΔH_f° −347 kJ mol^{-1}.

▷ Oxidiser.

Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 442 (*rev, bibl*)
Burns, J.H., *Acta Crystallogr.*, 1962, **15**, 89 (*cryst struct*)
Boyd, G.E. *et al*, *J. Chem. Eng. Data*, 1962, **7**, 237 (*synth, thermodynamics*)
Kondilenko, I.I. *et al*, *Opt. Spektrosk.*, 1975, **38**, 689 (*raman*)
Masaguer, J.R. *et al*, *J. Chem. Thermodyn.*, 1976, **8**, 525 (*thermochem data*)

BrNNiO IC-001717

Bromonitrosylnickel

$[Ni(NO)Br]_n$

M 168.6
Probably has polymeric or cluster struct. Dark green-black solid. Cl and I analogues known.

Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1940, **244**, 23.
Jahn, A., *Z. Anorg. Allg. Chem.*, 1959, **301**, 301 (*ir*)

BrNO IC-001718

Nitrosyl bromide

[13444-87-6]

BrNO

M 109.9
Interatomic distances: Br—N 214, N—O 115 pm; angle: BrNO 114°. Dissociates reversibly to Br_2 + NO (7% at r.t.). Synth. from NO_2 + KBr. Red gas, rapidly hydrol. to NO_2, HNO_2, NO and HBr. Dec. on warming. Bp ~0°.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, *Part* 2, 1967, **8/II**, 409 (*rev*)
Inorg. Synth., 1968, **11**, 194 (*synth, ir*)
Miller, D.J. *et al*, *Trans. Faraday Soc.*, 1970, **66**, 2414 (*struct*)
Braun, G., *Handbuch Prap. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 476 (*synth*)

$BrNO_2$ IC-001719

Bromine nitrite

Nitrato bromide. Nitryl bromide, 10CI

O=NOBr

M 125.9
Formed from Nitryl bromide, IC-001720 + hν in Ar matrix.

Tevault, D.E., *J. Phys. Chem.*, 1979, **17**, 2217 (*synth, ir*)

$BrNO_2$ IC-001720

Nitryl bromide

[13536-70-4]

M 125.9
Formed from NO_2 + Br in an Ar matrix.

Feuerhahn, M. *et al*, *J. Mol. Spectrosc.*, 1979, **77**, 429 (*synth, ir*)
Tevault, D.E., *J. Phys. Chem.*, 1979, **17**, 2217 (*synth, ir*)

$BrNO_3$ IC-001721

Bromine(I) nitrate

Nitryl hypobromite

[40423-14-1]

$BrONO_2$

M 141.9
Synth. from BrCl + $ClONO_2$ at −70°. Yellow liq. dec. into Br_2, NO_2 and O_2. Mp −42°. Dec. ~0°.

Schmeisser, M. *et al*, *Chem. Ber.*, 1961, **94**, 1533 (*rev, synth*)
Jolly, W.M., *Prep. Inorg. React.*, 1964, **1**, 246 (*synth*)
Brauer, G., *Handbuch Prap. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 340 (*synth*)

$BrNO_3$ IC-001722

Bromyl nitrate

O_2BrONO_2

M 173.9
Formed from $BrONO_2$ + O_3 in $CFCl_3$ at −78°. Orange solid. Dec. at low temp. to Br_2 + NO_2 + O_2.

Schmeisser, M. *et al*, *Chem. Ber.*, 1961, **94**, 1533 (*synth, structure*)
Schack, C.J. *et al*, *Inorg. Chem.*, 1974, **13**, 2378 (*synth*)
Brauer, G., *Handbuch Prap. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 346 (*synth*)

BrNS IC-001723

Thiazyl bromide ((SN)Br), 11CI

[52509-85-0]

BrS≡N

M 125.9
Formed by pyrolysis of $[S_4N_3]Br$. Isol. and characterised in an Ar matrix, one electron occupying the π^* orbital of the SN radical.

Peake, S.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 859 (*matrix isol, ir*)

BrN_3 IC-001724

Bromine azide (Br(N$_3$)), 11CI

Azido bromide

[13973-87-0]

BrN=N=N

M 121.9

Formed from AgN_3 + Br_2 in Et_2O. Orange-red liq. Mp −45°.

▷ Highly explosive. EF9200000.

Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, **1**, 476, 480 (*synth*)

Dehnicke, K., *Adv. Inorg. Chem. Radiochem.*, 1983, **26**, 169 (*rev*)

BrN_3O_9 IC-001725

Bromine(*III*) nitrate

Bromine trinitrate

Br(ONO$_2$)$_3$

M 265.9

Synth. from BrF_3 + $3N_2O_5$ or from BrF_3 + $3HNO_3$. Pale yellow solid, readily hydrol. Slowly dec. above 0° to Br_2 + O_2 + NO_2. Sol. CCl_4, freon. Mp 48° dec.

Schmeisser, M. *et al*, *Angew. Chem.*, 1961, **73**, 388 (*rev, synth*)

Jolly, W.M., *Prep. Inorg. React.*, 1964, **1**, 162 (*synth*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 341 (*synth*)

BrN_4OP IC-001726

Phosphorodiazidic bromide, 10CI

Diazidobromophosphine oxide

Diazidobromooxophosphorus(V)

[69715-82-8]

(N$_3$)$_2$P(O)Br

M 210.9

Not purif. Synth. from $POBr_3$ + NaN_3/MeCN.

▷ Presumed explosive.

Dillon, K.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1978, **14**, 511 (*synth, P-31 nmr*)

BrN_4P IC-001727

Phosphorodiazidous bromide, 10CI

Diazidobromophosphine. Diazidobromophosphorus(III)

[69715-78-2]

(N$_3$)$_2$PBr

M 194.9

Not purif. Synth. from PBr_3 + NaN_3/MeCN.

▷ Presumed explosive.

Dillon, K.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1036 (*synth, P-31 nmr*)

BrN_4PS IC-001728

Phosphorodiazidothioic bromide, 10CI

Diazidobromophosphine sulfide. Diazidobromothiooxophosphorus(V)

[69715-80-6]

(N$_3$)$_2$P(S)Br

M 226.9

Not purif. Synth. from $PSBr_3$ + NaN_3/MeCN.

▷ Presumed explosive.

Dillon, K.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1978, **14**, 511 (*synth, P-31 nmr*)

BrNa IC-001729

Sodium bromide (NaBr), 8CI

[7647-15-6]

NaBr

M 102.8

NaCl struct. Synth. by neutralisation of NaOH or Na_2CO_3 with aq. HBr initially as dihydrate. Commercially available. Hygroscopic colourless cubic cryst. V. sol. H_2O (116 g per 100 cm^3 at 50°; 121 g per 100 cm^3 at 100°). Mp 747°. Bp 1390°. ΔH_f° −361.4 kJ mol^{-1}; ΔG_f° −349.3 kJ mol^{-1}; S° 86.8 JK^{-1} mol^{-1}.

▷ Irritant. VZ3150000.

Dihydrate: [13466-08-5].

Cryst. from aq. solns. of NaBr. Colourless monoclinic cryst. Dec. on heating with H_2O loss (−2H_2O at 51°). V. sol. H_2O (79 g per 100 cm^3 at 25°). ΔH_f° −952 kJ mol^{-1}; ΔG_f° −828 kJ mol^{-1}; S° 179 JK^{-1} mol^{-1}.

Swanson, H.E. *et al*, *Natl. Bur. Std. Circ. (U.S.)*, 1954, **3**, 47 (*cryst struct*)

Lecomte, J., *Boll. Sci. Fac. Chim. Ind. Bologna*, 1963, **21**, 51; *CA*, 1964, **60**, 4956d (*ir*)

Haaf, W.R. *et al*, *Acta Crystallogr.*, 1964, **17**, 730 (*cryst struct, dihydrate*)

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 150 (*rev, bibl*)

Bonera, G. *et al*, *Phys. Rev.*, 1968, **165**, 391 (*Br-81 nmr*)

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **21**, 224 (*rev*)

Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 447 (*thermodyn*)

Tabeta, R. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3134B (*haz*)

$BrNaO_3$ IC-001730

Sodium bromite

Sodium bromate(III). *Bromic*(III) *acid, sodium salt. Bromous acid, sodium salt, 8CI*

[7486-26-2]

NaBrO$_2$

M 134.8

Desizing agent. Selective reagent for the oxidation of sulfides and alcohols. Unstable, readily dec. releasing O_2. Partially stabilised by cocrystallisation with NaOH. V. sol. H_2O (28 g per 100 cm^3 at 0°; 91 g per 100 cm^3 at 100°); insol. EtOH.

Trihydrate:

BrH_4NaO_5 M 188.9

Cryst. from aq. 2*M* NaOH soln. containing $NaBrO_2$. Commercially available. Mild oxidising agent. Colourless cryst. Dehydrates at r.t. *in vacuo* to give anhyd. $NaBrO_2$.

Djega-Mariadassou, G. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 2726 (*ir*)

Gmelin Handbook Inorg. Chem., System No. 21, 1970, **5**, 1802 (*rev, bibl*)

Kageyama, T. *et al*, *Nippon Kagaku Kaishi (J. Chem. Soc. Jpn.)*, 1972, 1064; *CA*, **77**, 66861 (*stability*)

Kageyama, T. *et al*, *Synthesis*, 1983, 815 (*synth, uses, anhyd. trihydrate*)

Japan. Pat., 59 207 804, (1984); *CA*, 1985, **102**, 97731 (*synth, trihydrate*)

Okawara, M., *Yuki Gosei Kagaku Kyokaishi*, 1984, **42**, 751; *CA*, **101**, 158406 (*rev, bibl*)

Japan. Pat., 60 186 582, (1985); *CA*, 1986, **104**, 189236 (*stabilisation*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3134C (*haz*)

$BrNaO_3$ IC-001731

Sodium bromate(*V*)

Bromic(V) *acid, sodium salt, 8CI*

[7789-38-0]

NaBrO$_3$

M 150.8

Isostructural with $NaClO_3$. Manuf. by electrolysis of aq. NaBr. Synth. (with NaBr) by adding bromine to aq. NaOH. Also prepared by mixing aq. solns. of Na_2SO_4 and $Ba(BrO_3)_2$. Commercially available. Component of oxidising solns. Used to set hair. Component of the Belousov-Zhabotinskii oscillating reaction (malonic acid, H_2SO_4, $Ce_2(SO_4)_3$, [or $[Fe(bipy)_3]^{2\oplus}$] and $NaBrO_3$). Colourless cubic cryst. Dec. on heating with O_2 evolution and formation of NaBr. V. sol. H_2O (28 g per 100 cm^3 at 0°; 91 g per 100 cm^3 at 100°); insol. EtOH. ΔH_f° −334 kJ mol^{-1}; ΔG_f° −243 kJ mol^{-1}; S° 129 JK^{-1} mol^{-1}.

▷ Oxidiser, irritant. EF8750000.

Figgis, B.N. *et al*, *Proc. R. Soc. London, A*, 1962, **269**, 469 (*O-17 nmr*)

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1970, **5**, 1803 (*rev, bibl*)

Sterzel, W. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **383**, 231 (*ir*)

Kondilenko, I.I. *et al*, *Opt. Spektrosk.*, 1975, **38**, 689 (*raman*)

Abrahams, S.C. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 3601 (*cryst struct*)

Bachelart, S. *et al*, *CA*, 1982, **96**, 149841 (*oscillating reaction*)

Oldfield, E. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 919 (*Na-23 nmr*)

Kovalenko, A.S. *et al*, *Teor. Eksp. Khim.*, 1985, **21**, 669 (*oscillating reaction*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3134A (*haz*)

$BrNbO_2$ IC-001732

Niobium(*V*) bromide oxide ($NbBrO_2$), 11CI

Niobium bromide dioxide

[103124-85-2]

NbO$_2$Br

M 204.8

Synth. by heating Nb foil, Nb_2O_5 and Br_2 in a sealed tube at 450/400°. Yellow solid. Dec. at 500° to Nb_2O_5 and $NbOBr_3$.

Schaefer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1986, **534**, 209 (*synth, props*)

BrNbSe IC-001733

Niobium bromide selenide (NbBrSe), 10CI

[79845-45-7]

NbBrSe

M 251.7

Struct. probably analogous to corresp. iodide (Niobium iodide selenide (NbISe), IC-020182), with cube-like core. Synth. by heating Nb_2Br_5, Nb and Se to 800°. Cryst.

Fedorov, V.E. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 1447 (*synth, cryst struct, dia*)

BrO IC-001734

Bromine oxide (BrO), 11CI

[15656-19-6]

[Br—O]

M 95.9

Free radical, studied in vapour phase. Formed by flash photolysis of $BrO_2^\ominus$. Dec. to Br_2 + O_2.

Clyne, M.A.A. *et al*, *Trans. Faraday Soc.*, 1966, **62**, 1175 (*reactions*)

Barat, F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 1485 (*synth*)

Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1384 (*rev*)

BrOP IC-001735

Phosphenous bromide, 10CI

Bromooxophosphorus(III). *Phosphorus bromide oxide (PBrO), 8CI. Bromooxophosphine*

BrP=O

M 126.8

Calc. interatomic distance: P=O 143.9 pm; est. angle BrPO 110°. Synth. from PBr_3—O_2 mixt. over Ag at 825°. Isol. in Ar matrix. Also may be formed during part. hydrol. of PBr_3 in vapour phase. Reactive, unstable sp. of low coordination number.

Binneweis, M. *et al*, *High Temp. Sci.*, 1986, **22**, 83 (*synth, ms*)

Schnöckel, H. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **548**, 161 (*formn, ir*)

Schunck, S. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **579**, 66 (*synth, reaction*)

BrOPu IC-001736

Plutonium(*III*) bromide oxide (PuBrO)

Plutonium(III) *oxobromide*

[49788-72-9]

PuOBr

M 334.9

8-Coordinate, with the PbFCl struct. Synth. from PuO_2 + HBr at 750°. Green solid. Insol. H_2O; sol. dil. acid. ΔH_f −867 kJ mol^{-1}.

Zachariasen, W.H., *Acta Crystallogr.*, 1949, **2**, 388 (*cryst struct*)

Weigel, F. *et al*, *J. Less-Common Met.*, 1982, **84**, 147 (*thermodyn*)

Fuger, J., *ACS Symp. Ser.*, 1983, **216**, 75 (*synth*)

BrOTl IC-001737

Thallium(*III*) bromide oxide (TlBrO)

Thallium oxide bromide. Thallium oxybromide

[14922-04-4]

Tl(OBr)

M 300.2

Isostructural with InOBr (FeOCl). Synth. from $TlBr_3$ + O_3; Tl_2CO_3 + (l) Br_2. Luminescent substance for identifying screens for radiography. Solid, dec. at 230° to give Tl_2O, O_2, Br_2. Forms solid solns. with lanthanum and lead oxybromides.

▷ Highly toxic.

Kauffmann, V.S. *et al*, *Z. Anorg. Allg. Chem.*, 1966, **347**, 318 (*synth*)

Ger. Pat., 2 461 260, (1976) (*use*)

Günter, J.R., *Z. Anorg. Allg. Chem.*, 1978, **438**, 203 (*struct*)

BrOV IC-001738

Vanadium(*III*) bromide oxide (VBrO)

Bromooxovanadium(III)

[13520-88-2]

VOBr

M 146.8

Struct. comprises *trans*-VO_4Br_2 octahedra: all of the atoms are shared; O with 4V, Br with 2V. Synth. from excess VBr_3 and As_2O_3 in a sealed tube at 400°. Various species, including Li, ferrrocene and pyridines may be intercalated. Violet solid.

Li intercalate:

BrLiOV M 153.7

From parent compd. + LiBu or by electrolysis. Cathode in Li batteries. Actual composition $Li_{0.8}VOBr$.

Levayer, C. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 167 (*synth, cryst struct*)

Armand, M. *et al, J. Power Sources*, 1978, **3**, 137 (*lithiation*)

Rouxel, J. *et al, Rev. Chim. Minér.*, 1982, **19**, 317 (*intercalation*)

BrOZr IC-001739

Zirconium bromide oxide (ZrBrO), 11Cl

[87335-97-5]

ZrBrO

M 187.1

Non-stoichiometric with respect to oxygen over the range $BrOZr$ to $BrO_{0.45}Zr$. The ZrBr struct. is retained with oxide in distorted tetrahedral sites between the Zr layers, with random occupancy (ZrBr has the layer sequence Br—Zr—Zr—Br). Synth. by heating ZrO_2 and ZrBr in a sealed tantalum container typically at 1025° for 7 days. Bronze solid.

Seaverson, L.M. *et al, Inorg. Chem.*, 1983, **22**, 3202 (*synth, cryst struct*)

BrO_2 IC-001740

Bromine oxide (BrO_2), 10Cl, 9Cl

Bromine dioxide

[21255-83-4]

$[BrO_2]_n$

M 111.9

Probably polymeric as solid. Synth. from $Br_2 + O_3$ in $CFCl_3$ at −30° Dark-yellow solid. Dec. at 0° to $Br_2 + O_2$.

▷ May explode if heated rapidly.

Dimer: see Bromine oxide (Br_2O_4), IC-001870

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, Part 1, 1958, **2/II**, 748 (*rev*)

Schmeisser, M. *et al, Adv. Inorg. Chem. Radiochem.*, 1963, **5**, 71 (*rev*)

Downs, A.J. *et al, Compr. Inorg. Chem.*, 1973, **2**, 1361 (*rev*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 317 (*comb*)

BrO_5Ta IC-001741

Tantalum(*V*) bromide oxide ($TaBrO_5$), 11Cl

[14118-77-5]

TaO_2Br

M 292.8

Synth. from Ta + Ta_2O_5 + Br_2 in a temp. gradient (500-400°). Used in photochromic plastics. Gold-orange solid.

Netherlands Pat., 6 511 295, (1966); *CA*, **65**, 6572b (*use*)

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1986, **534**, 209 (*synth, struct*)

BrO_2U IC-001742

Uranium bromide oxide ($UBrO_2$)

Bromodioxouranium(V)

[26512-08-3]

UO_2Br

M 349.9

U 7-coord. within a pentagonal bipyramid of 2Br + 5O. Synth. from UO_2Br_2 at 650° or from UO_2Cl_2 + HBr. Moisture-sensitive dark brown solid. Insol. H_2O. Paramagnetic, $\mu_{eff} = 1.76\mu_B$ ($\theta = -200$K). Dec. > 400°.

Prigent, J. *et al, Bull. Soc. Chim. Fr.*, 1962, 406 (*synth*)

Levet, J.C., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **260**, 4775 (*synth, magnetism*)

Levet, J.C., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 703 (*synth, magnetism*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1222 (*synth*)

Levet, J.C. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2542 (*cryst struct*)

Thibaut, E. *et al, J. Am. Chem. Soc.*, 1982, **104**, 5266 (*pe*)

BrO_3 IC-001743

Bromine oxide (BrO_3)

Bromine trioxide

[32062-14-9]

BrO_3

M 127.9

Radical species isolated in matrices, unstable above 130K. BrO_3 pyramid is considerably flattened in comparison to $BrO_3^{\ominus}$. Formed by irradiation of $BrO_3^{\ominus}$ at low temp.

Begum, A. *et al, J. Chem. Soc. A*, 1970, 918.

Amichai, O. *et al, J. Phys. Chem.*, 1970, **74**, 3670 (*uv, vis*)

Rao, K.V.S. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 147 (*esr*)

Byberg, J.R., *J. Chem. Phys.*, 1985, **83**, 919.

BrO_3Rb IC-001744

Rubidium bromate(*V*)

Bromic acid, rubidium salt, 8CI

[13446-70-3]

$RbBrO_3$

M 213.3

Isotypic with $KBrO_3$. Prepd. by slow neutralisation of Rb_2CO_3 using $HBrO_3$ in aq. soln. Colourless rhombohedral cryst. Mod. sol. H_2O (2.9 g per 100 cm^3 at 25°; 5.1 g per 100 cm^3 at 40°). Mp 430°. ΔH_f° −367 kJ mol^{-1}; ΔG_f° −278 kJmol^{-1}; S° 161 J K^{-1} mol^{-1}.

Gmelin Handbook Inorg. Chem., Syst. No. 24, 1955, 180 (*rev, bibl*)

Swanson, H.E. *et al, Natl. Bur. Std. Circ. (U.S.)*, No. 539, 1959, 8, 45 (*cryst struct*)

Shklovskaya, R.M. *et al, Metody Poluch. Khim. Reakt. Prep.*, 1967, **16**, 77; *CA*, 1968, **69**, 48786 (*synth*)

Kondilenko, I.I. *et al, Opt. Spektrosk.*, 1975, **38**, 689 (*raman*)

BrO_3Re IC-001745

Rhenium(*VII*) bromide oxide ($ReBrO_3$)

Rhenium bromide trioxide

[13350-30-6]

$ReBrO_3$

M 314.1

Molecular. Synth. from (i) Br_2 and $KReO_4$ (ii) ReO_3 and Br_2. Colourless hygroscopic liq., said to dec. to ReO_3 on heating.

Bruckl, A. *et al, Monatsh. Chem.*, 1933, **63**, 329 (*synth, props*)

Colton, R. *et al, Chem. Ind. (London)*, 1959, 1314 (*synth, props*)

Miller, F.A. *et al, Spectrochim. Acta*, 1960, **16**, 1148 (*ir*)

BrO_3Tl IC-001746

Thallium(*I*) bromate ($Tl(BrO_3)$)

$Tl[BrO_3]$

M 332.2

Solid, dec. at 120° to Tl_2O_3, Br_2, O_2. Sl. sol. H_2O (0.49 g per 100 cm^3 at 30°). ΔH_f° −136.4 kJ mol^{-1}; ΔG_f° −53.1 kJ mol^{-1}.

▷ Highly toxic.

Khoo, K.H., *J. Inorg. Nucl. Chem.*, 1968, **30**, 2425; 1969, **31**, 9437.

BrO_4Rb IC-001747

Rubidium perbromate ($RbBrO_4$)

Rubidium bromate(VII). *Bromic*(VII) *acid, rubidium salt. Perbromic acid, rubidium salt, 8CI*

[24402-68-4]

$RbBrO_4$

M 229.3

Perbromates were first obtained by radioactive β decay of ^{83}Se to ^{83}Br. Isotypic with $BaSO_4$. Prepd. by oxidation of $RbBrO_3$ with XeF_2 in aq. soln. Also obt. by neutralisation of $HBrO_4$, prepd. by preparative ion-exchange chromatography, with an aq. soln. of RbOH. Colourless orthorhombic cryst. V. sol. H_2O. Dec. at 291°.

▷ Oxidiser.

Appelman, E.H., *J. Am. Chem. Soc.*, 1968, **90**, 1900 (*synth*)

Brown, L.C. *et al, J. Am. Chem. Soc.*, 1969, **91**, 2250 (*ir, raman*)

Tytov, L.G. *et al, Zh. Neorg. Khim.*, 1986, **31**, 589 (*synth, cryst struct*)

BrPS IC-001748

Phosphenothious bromide

Bromothioxophosphorus(III). *Phosphorus bromide sulfide (PBrS). Bromothioxophosphine*

BrP=S

M 142.9

Synth. on passing $PSBr_3$ over Ag at 525°. Isol. in Ar matrix. Reactive, unstable sp. of low coordination number.

Bürgwies, M. *et al, Z. Anorg. Allg. Chem.*, 1987, **552**, 147 (*formn, str*)

Schöckel, H. *et al, Z. Anorg. Allg. Chem.*, 1987, **552**, 155 (*synth, ir*)

BrRb IC-001749

Rubidium bromide (RbBr), 8CI

[7789-39-1]

RbBr

M 165.3

NaCl struct. Prepd. by slow neutralisation of Rb_2CO_3 with HBr in aq. soln. Alternatively, reaction of Rb_2CO_3 with Br_2 in aq. soln. containing $N_2H_4.H_2O$ affords pure RbBr. Commercially available. Colourless cubic cryst. V. sol. H_2O (98 g per 100 cm^3 at 5°; 205 g per 100 cm^3 at 114°); spar. sol. Me_2CO; insol. EtOH. Mp 693°. Bp 1340°. ΔH_f° −395 kJ mol^{-1}; ΔG_f° −382 kJ mol^{-1}; S° 110 J K^{-1} mol^{-1}.

Gmelin Handbook Inorg. Chem., Syst. No. 24, 1955, 162 (*rev, bibl*)

Deshpande, V.T. *et al, Acta Crystallogr.*, 1961, **14**, 353 (*cryst struct*)

Vulich, A.I. *et al, CA*, 1969, **70**, 53444 (*synth*)

BrSSb IC-001750

Antimony bromide sulfide (SbBrS), 9Cl, 8CI

Bromothioxostibine. Bromothioxoantimony(III)

[14794-85-5]

BrSb=S

M 233.7

Orthorhombic (at r.t.). The Sb is 7 coordinated by Br (×4) and S (×3) (Sb—Br 293.7, 363.3, Sb—S 247.3-267.1 pm) forming pleated chains of $(Sb)_n^{n\oplus}$ between which are the $Br^{\ominus}$ anions. Synth. from Sb + S + Br_2, or from Sb_2S_3 + $SbBr_3$ in Br_2 at 200-285° and 30-270 atm. Orange prisms or needles. Mp 330° dec. Photoconductive and ferroelectric. Undergoes phase transitions at −95° and −182°. Dec. at Mp → Sb_2S_3 + $SbBr_3$. Exhibits anomalous electrooptical and electromechanical props. under visible light.

Gmelin Handbook Inorg. Chem., Syst. No. 18, 1949, 549 (*rev, bibl*)

Chepur, D.V. *et al, Phys. Status Solidi*, 1968, **30**, 461 (*ir*)

Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1969, **14**, 312 (*synth*)

Litvin, B.N. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1970, **6**, 375; *Inorg. Materials (Engl. Transl.)*, 1970, **6**, 308 (*synth*)

Popolitov, V.I. *et al, Phys. Status Solidi A*, 1970, **3**, K1 (*synth*)

Aleksandrov, A.Y. *et al, Kristallografiya*, 1972, **17**, 332; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1972, **17**, 281 (*mössbauer*)

Semin, G.K., *Phys. Status Solidi A*, 1972, **11**, K61 (*ngr*)

Inorg. Synth., 1973, **14**, 160 (*synth*)

Teng, M.K. *et al, Phys. Status Solidi B*, 1974, **62**, 173 (*raman*)

Furman, E. *et al, Phys. Rev. B: Solid State*, 1976, **13**, 1703 (*raman*)

Inushima, T. *et al, Ferroelectrics*, 1981, **38**, 885 (*raman*)

Inushima, T. *et al, Phys. Rev. B: Solid State*, 1982, **26**, 2525 (*struct*)

Popolitov, V.I. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1983, **19**, 1651; *Inorg. Materials (Engl. Transl.)*, 1983, **19**, 1459 (*synth*)

Inushima, T. *et al, Jpn. J. Appl. Phys., Part 1*, Suppl 24-2, 1985, **24**, 600 (*cryst struct*)

Siapkas, D. *et al, Z. Kristallogr.*, 1986, **175**, 305 (*ir, cryst struct*)

BrSTl IC-001751

Thallium(*III*) bromide sulfide (TlBrS)

Thallium(III) *sulfide bromide. Thallium*(III) *thiobromide*

[13595-94-3]

TlSBr

M 316.3

Tetragonal, isostructural with PbFCl. Synth. from TlBr + S at 180° in sealed tube (30 hr). Solid, dec. with alkalis and hot acids; purif. by zone refining. Insol. H_2O, org. solvs. Mp 120°.

▷ Highly toxic.

Batsanov, S.S. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 1355 (*synth*)

Batsanov, S.S. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 143; *Inorg. Materials (Engl. Transl.)*, 1968, **4**, 117.

Filatkina, V.S. *et al, Zh. Neorg. Khim.*, 1969, **14**, 2288 (*struct*)

IC-001752

BrS_2Ta

Tantalum(*V*) bromide sulfide ($TaBrS_2$), 11CI

[82546-48-3]

$TaBrS_2$

M 324.9

Struct. unknown. Synth. by disproportionation of Tantalum(*V*) bromide sulfide ($TaBr_3S$), IC-001985 at 170°. Black solid.

bin Baba, I., *Sains Malays.*, 1981, **10**, 29 (*synth, ir*)

IC-001753

BrSbSe

Antimony bromide selenide (SbBrSe), 9CI, 8CI

Bromoselenoxostibine. Bromoselenoxoantimony(III)

[19445-24-0]

BrSb=Se

M 280.6

Orthorhombic. Synth. from Br + Sb + Se in gas phase; or solvo-thermally at 210-300°/30-290 atm. in Br_2 or HBr. Black needles. Mp 250°. Photoelectric.

Klazar, J. *et al, Collect. Czech. Chem. Commun.*, 1968, **33**, 973 (*synth, props*)

Horák, J. *et al, Krist. Tech.*, 1968, **3**, 241 (*synth, photoelectric props*)

Chepur, D.V. *et al, Phys. Status Solidi*, 1968, **30**, 461 (*ir*)

Popolitov, V.I., *Kristallografiya*, 1969, **14**, 375; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1969, **14**, 312 (*synth*)

Popolitov, V.I. *et al, Phys. Status Solidi A*, 1970, **3**, K1 (*synth*)

IC-001754

BrSeTl

Thallium(*III*) bromide selenide (TlBrSe)

Thallium selenide bromide. Thallium(III) *selenobromide*

TlSeBr

M 363.2

Two forms identified depending on prep. Two synth. methods: (i) TlBr + Se at 280° in sealed tube (40 hr), (ii) Tl + Se_2Br_2 at 280°, sealed tube (140 hr). This method gives a product containing Tl(*I*). Solid, dec. with alkalis and hot acids; purif. by zone refining. Insol. H_2O, org. solvs. Mp 220°.

▷ Highly toxic.

Batsanov, S.S. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1966, **167**, 89; 1964, **158**, 1355 (*synth*)

Batsanov, S.S. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 143; *Inorg. Materials* (*Engl. Transl.*), 1968, **4**, 117.

IC-001755

$BrSe_2Ta$

Tantalum(*V*) bromide selenide ($TaBrSe_2$), 11CI

[82546-49-4]

$TaBrSe_2$

M 418.7

Struct. unknown. Synth. by disproportionation of Tantalum(*V*) bromide selenide ($TaBr_3Se$), IC-001988 at 180°. Black solid.

bin Baba, I., *Sains Malays.*, 1981, **10**, 29 (*synth, ir*)

IC-001756

$BrTe_2$

Tellurium bromide (Te_2Br)

Ditellurium bromide. Tellurium subbromide

[12514-37-3]

Te_2Br

M 335.1

Polymeric chain-type struct. with bridging Br atoms. Formed from Te + Br_2 at 300°. Grey needles, stable in air.

Rabenau, A. *et al, Angew. Chem.*, 1970, **82**, 811 (*synth*)

Kniep, R. *et al, Z. Anorg. Allg. Chem.*, 1976, **422**, 17 (*cryst struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 11, 1978, **B3**, 2 (*bibl*)

IC-001757

BrTl

Thallium(*I*) bromide (TlBr)

[7789-40-4]

TlBr

M 284.2

Has CsCl struct., becomes metallic at high pressures. Synth. from acidified solns. of Tl(*I*) salts by addn. of $Br^{\ominus}$. Air-stable light-sensitive yellow solid. Spar. sol. H_2O. Mp ~460°. Bp 815°. Oxid. by Br_2 to $TlBr_3$.

▷ Highly toxic. XG3850000.

Samara, G.A. *et al, J. Chem. Phys.*, 1962, **37**, 408 (*conduct*)

Keneshea, F.J. *et al, J. Phys. Chem.*, 1965, **69**, 3910.

Alcock, N.W., *Acta Crystallogr., Sect. A*, 1969, **25**, S101 (*struct*)

Ladd, M.F.C. *et al, Trans. Faraday Soc.*, 1970, **66**, 2767.

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 876 (*synth*)

IC-001758

BrY

Yttrium bromide (YBr)

Yttrium monobromide

[17655-40-2]

YBr

M 168.8

Has ZrCl struct. with Y_6 octahedra linked into sheets. Synth. from YBr_3 + Y at 780-950°. Can be intercalated with Li. Black plates; chemiluminescent in vapour phase.

Mattausch, H. *et al, Inorg. Chem.*, 1980, **19**, 2128 (*synth, struct*)

Fischell, D.R. *et al, J. Chem. Phys.*, 1980, **73**, 4260 (*luminescence*)

Ford, J.E. *et al, Inorg. Chem.*, 1984, **23**, 2094 (*synth, use*)

IC-001759

BrZr

Zirconium bromide (ZrBr), 11CI

[31483-18-8]

ZrBr

M 171.1

Structure comprises slabs of four close-packed layers X—Zr—Zr—X, the slabs repeating (A,C,B) (*cf.* ZrCl where the repeat is ABC). Synth. by heating in a temp. gradient over several d. $ZrBr_4$ + Zr turnings in a sealed Ta ampoule. Behaves as a 2-D metal with conductivities ~55 ohm $^{-1}$ cm^{-1} parallel to sheets and 10^{-3} ohm^{-1} cm^{-1} perpendicular to sheets. Pauli paramagnetic; much harder than ZrCl. Black solid.

Daake, R.L. *et al, Inorg. Chem.*, 1977, **16**, 2029 (*synth, cryst struct, pe*)

Corbett, J.D., *Inorg. Chem.*, 1983, **22**, 2669 (*pe*)

Inorg. Synth., 1983, **22**, 26 (*synth, rev*)

IC-001760

$Br_2^{\oplus}$

Dibromine(1+)

[12595-71-0]

$Br_2^{\oplus}$

M 159.8 (ion)

Br—Br 215 pm. Forms scarlet salts. Dec. in H_2O.

Di-μ-fluorotetradecafluorotriantimonate(1−): [11088-93-0].

$Br_2F_{16}Sb_3$ M 829.0

Synth. from Br_2, $S_2O_6F_2$ and SbF_5. Moisture-sensitive bright red cryst. melts to give cherry red liq. V. sol. HSO_3F. Mp 85.5°, Mp 69°. $\mu_{eff} = 2.0\mu_B$ (80-300K). Ir ν 700s, sh, 655vs, 585w, 560w, 485m, 425w cm^{-1}.

Hexafluoroarsenate: [50960-75-3].

$AsBr_2F_6$ M 348.7

Edwards, A.J. *et al, J. Chem. Soc. A*, 1971, 2318 (*cryst struct, $Sb_3F_{16}^{\ominus}$*)

Gillespie, R.J. *et al, Advan. Raman Spectrosc.*, 1972, **1**, 364, 539 (*raman*)

Gillespie, R.J. *et al, Inorg. Chem.*, 1972, **11**, 586 (*synth, raman*)

Smalc, A., *CA*, 1973, **79**, 130321 (*$AsF_6^{\ominus}$*)

Belousova, E.V. *et al, Zh. Fiz. Khim.*, 1975, **49**, 1075 (*ir*)

Wilson, W.W. *et al, Inorg. Chem.*, 1980, **19**, 1489 (*synth, $Sb_3F_{16}^{\ominus}$*)

Harris, T. *et al, J. Mol. Spectrosc.*, 1983, **98**, 269 (*spectra*)

Van Lonkhuyzen, H. *et al, Chem. Phys.*, 1984, **89**, 313 (*uv*)

Van der Meer, W.J. *et al, Chem. Phys.*, 1987, **115**, 109 (*pe*)

IC-001761

Br_2Ca

Calcium bromide ($CaBr_2$), 8CI

Calcium dibromide

[7789-41-5]

$CaBr_2$

M 199.8

Isostructural with $CaCl_2$. Synth. by dehydration of hexahydrate at 250° under vacuum. Alternatively pure $CaBr_2$ prepd. by reaction of calcium metal dissolved in liq. NH_3 with NH_4Br. Commercially available. Component of drilling fluids. Constit. of photothermographic papers. Colourless orthorhombic deliquescent cryst. V. sol. H_2O (142 g per 100 cm^3 at 20°); sol. EtOH, Me_2CO; spar. sol. MeOH, $CH_2ClCOOH$ (2.5 g per 100 cm^3 at 94°). Mp 742°. ΔH_f° −683 kJ mol^{-1}; ΔG_f° −664 kJ mol^{-1}; S° 130 J K^{-1} mol^{-1}.

▷ EV9328000.

Monohydrate: [62648-72-0].

Br_2CaH_2O M 217.9

Hexahydrate: [13477-28-6].

$Br_2CaH_{12}O_6$ M 307.9

Cryst. from aq. solns. of $CaBr_2$. Heat storage material, normally used in conjunction with $CaCl_2.6H_2O$. Hygroscopic colourless hexagonal cryst. Dec. on heating with H_2O loss. V. sol. H_2O (594 g per 100 cm^3 at 0°; 1360 g per 100 cm^3 at 25°); sol. EtOH, Me_2CO. Mp 34.2°. ΔH_f° −2506 kJ mol^{-1}; ΔG_f° −2153 kJ mol^{-1}; S° 410 J K^{-1} mol^{-1}.

Gmelin Handbook Inorg. Chem., Syst. No. 28, 1957, **B2**, 584, 589 (*rev, bibl*)

Brackett, E.B. *et al, J. Inorg. Nucl. Chem.*, 1963, **25**, 1295 (*synth, cryst struct*)

Paul, R.C. *et al, J. Indian Chem. Soc.*, 1964, **41**, 541 (*soly*)

Malhotra, K.C. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 3767 (*soly*)

Hadenfeldt, C., *Z. Naturforsch., B*, 1975, **30**, 165 (*synth*)

Leclaire, A. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2938 (*hexahydrate, cryst struct*)

Smirnov, N.I. *et al, Teor. Eksp. Khim.*, 1977, **13**, 88 (*Br-79 nqr*)

Buzagh-Gere, E. *et al, Therm. Anal., Proc. Int. Conf., 5th, 1977*, 1977, 266; *CA*, 1978, **89**, 122327 (*hexahydrate, thermal dec*)

Scrosati, B., *Solubility Data Ser.*, 1980, **11**, 298, 339 (*soly*)

Vincent, C.A., *Solubility Data Ser.*, 1980, **11**, 78, 146, 243 (*soly*)

Farmer, R.M. *et al, Inorg. Nucl. Chem. Lett.*, 1981, **17**, 51 (*Ca-43 nmr*)

Al'tmann, A.B., *CA*, 1982, **96**, 75004 (*ed, struct*)

Chase, M.W. *et al, J. Phys. Chem. Ref. Data*, 1985, **14**, 461 (*thermochem data*)

Feilchenfeld, H. *et al, Solar Energy*, 1985, **34**, 199 (*hexahydrate, use*)

Br_2Cd

Cadmium bromide ($CdBr_2$) IC-001762

[7789-42-6]

$CdBr_2$

M 272.2

Has CdI_2 struct. in solid state; linear molecule in gas phase. Synth. from elements or from $CdCO_3$ and HBr. Colourless hygroscopic cryst. Sol. H_2O (57 g per 100 cm^3 at 10°), EtOH (26.6 g per 100 cm^3 at 15°), Me_2CO (1.34 g per 100 g at 18°). Mp 570°. Bp 863°.

▷ EU9935000.

Monohydrate: Cryst. (H_2O at > 36°).

Tetrahydrate: [13464-92-1].

Obt. by evap. of satd. aq. solns. of $CdBr_2$. Cryst. (H_2O at < 36°). Octahedral Cd (4 Br + 2 O). Dehydrates at 36° at 1 atm.

Gmelin Handbook Inorg. Chem., Syst. No. 33, 1959, 518 (*rev, bibl*)

Davies, J.E.D. *et al, J. Chem. Soc. A*, 1968, 2054 (*soln raman*)

Lyskovich, A.B. *et al, Izv. Akad. Nauk SSSR, Ser. Fiz.*, 1974, **38**, 1299 (*opt prop, photo cond, luminescence*)

Babushkina, T.A. *et al, Koord. Khim.*, 1975, **1**, 1266 (*nqr*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1041 (*synth*)

Haberkorn, R.A. *et al, Inorg. Chem.*, 1976, **15**, 2408 (*Cd-113 nmr, soln*)

Leligny, H. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 5 (*cryst struct, tetrahydrate*)

Nolle, A., *Z. Naturforsch., A*, 1978, **33**, 666 (*Cd-113 nmr, solid*)

Givan, A. *et al, J. Chem. Phys.*, 1980, **72**, 3809 (*ir, raman in matrix*)

Anderson, A. *et al, Spectrosc. Lett.*, 1981, **14**, 105 (*ir, raman, solid*)

Bristow, D.J. *et al, Chem. Phys.*, 1983, **75**, 263 (*pe*)

Campbell, J.A. *et al, J. Phys. C*, 1983, **16**, 999 (*ir*)

Dovgii, Ya.O. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1985, **21**, 864 (*optical prop*)

Mioc, U.B. *et al, Thermochim. Acta*, 1985, **84**, 239 (*thermal dec, dihydrate*)

Petrov, V.M. *et al, Zh. Strukt. Khim.*, 1985, **26**, 52 (*ed*)

Chaudhary, S.K. *et al, Acta Crystallogr., Sect. B*, 1987, **43**, 225 (*struct*)

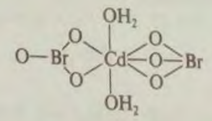
Churagulov, B.R. *et al, Zh. Fiz. Khim.*, 1987, **61**, 2507 (*$CdBr_2/H_2O$ system*)

$Br_2CdH_4O_8$ IC-001763

Diaquadibromatocadmium

Cadmium bromate dihydrate. Diaqua(bromato-O,O′) cadmium(1+) bromate, 10CI

[81283-08-1]



M 404.2

7-Coordinate Cd. Needles.

Murty, V.V.S. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1978, **148**, 158.

Murty, V.V.S. *et al, Indian J. Phys., A*, 1981, **55**, 310 (*synth, cryst struct*)

IC-001764

$Br_2CdH_6N_2$

Diamminedibromocadmium(*II*)

Cadmium(II) bromide diammoniate

[33071-85-1]

$CdBr_2(NH_3)_2$

M 306.2

Polymeric with octahedral Cd. Colourless solid. Forms a dihydrate.

MacGillavry, C.H. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1936, **94**, 231 (*struct*)
Clark, R.J.H. *et al*, *J. Chem. Soc. A*, 1966, 1425 (*ir*)
Patil, K.C. *et al*, *Can. J. Chem.*, 1971, **49**, 3831 (*synth, thermal anal, ir*)
Chalmers, R.A. *et al*, *Chim. Anal. (Bucharest)*, 1971, **1**, 42 (*synth*)
Kokozei, V.N. *et al*, *Ukr. Khim. Zh. (Russ. Ed.)*, 1987, **53**, 1014; *C.A.*, 1988, **108**, 179058 (*synth, ir*)

IC-001765

Br_2CdO_6

Cadmium bromate ($Cd(BrO_3)_2$)

[14518-94-6]

$Cd(BrO_3)_2$

M 368.2

Obt. by dehydration of hydrate. Cryst. Sol. H_2O (125 g per 100 cm^3).

Dihydrate: [19320-65-1]. *Diaquabis(bromato-O)cadmium*
Synth. from $CdSO_4$ and $Ba(BrO_3)_2$ in aq. soln. Cryst. Coordination sphere of Cd has 7 near O (5 O from pyramidal BrO_3 groups and $2OH_2$) and one further weaker O. Dehydrates at *ca.*125°; dec. at 140° *in vacuo*.

[70341-04-7]

Gmelin Handbook Inorg. Chem., Syst. No. 33, 1959, 542 (*rev, bibl*)
Dušek, B. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 307 (*thermal anal, dihydrate*)
Golovastikov, N.I., *Kristallografiya*, 1979, **24**, 259 (*cryst struct, dihydrate*)
Murty, V.V.S. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1979, **148**, 158 (*cryst struct, dihydrate*)
Gavanda, A.M. *et al*, *Indian J. Chem., Sect. A*, 1982, **21**, 287 (*thermal dec*)
Ramaprabhu, S. *et al*, *Pramana*, 1984, **23**, 141 (*Br-79 nqr, dihydrate*)
Sasidher, Y.U. *et al*, *J. Mol. Struct.*, 1986, **147**, 113 (*synth, pmr, dihydrate*)
Devanathan, T. *et al*, *J. Raman Spectrosc.*, 1987, **18**, 525 (*ir, raman, dihydrate*)
Devanathan, T. *et al*, *J. Solid State Chem.*, 1988, **74**, 184 (*synth, ir, raman, powder structs*)

IC-001766

Br_2Cf

Californium(*II*) bromide ($CfBr_2$)

Californium dibromide

[36700-18-2]

$CfBr_2$

M 411.8

Isostructural with $EuBr_2$ ($SrBr_2$) with 8-coord. Cf. Synth. from $CfBr_3 + H_2$ (650°). Red-amber solid.

[60188-17-8]

Peterson, J.R. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 423 (*synth, struct*)

IC-001767

$Br_2Cl^{\ominus}$

Bromochlorobromate(*I*)(1−)

[16871-87-7]

$[Br—Br—Cl]^{\ominus}$

M 195.2 (ion)

Linear ion. Forms red salts. Dissociates in H_2O.

K salt: [60346-72-7].
Cs salt: [22325-19-5].
Br_2ClCs M 328.1
Synth. from CsCl, Br_2 and HCl in H_2O. Coarse bright orange anisotropic cryst. Loses Br_2 at r.t.
Rb salt: [36491-26-6].
Br_2ClRb M 280.7
Synth. from RbCl, Br_2 and HCl in H_2O.

Bell, B.P. *et al*, *J. Chem. Soc. A*, 1966, 1607 (*formn const*)
Breneman, G.L. *et al*, *Acta Crystallogr.*, 1967, **23**, 334 (*cryst struct*)
Ault, B.S. *et al*, *J. Chem. Phys.*, 1974, **64**, 4853 (*ir, raman, K salt*)
Andrews, L. *et al*, *Inorg. Chem.*, 1980, **19**, 463 (*ir, raman*)
Miroonenko, A.P. *et al*, *Zh. Neorg. Khim.*, 1982, **27**, 1043; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 586 (*synth, Cs, Rb salts*)

IC-001768

Br_2ClOP

Phosphoryl bromide chloride ($POBr_2Cl$), 9Cl, 8Cl

Dibromochlorophosphine oxide.
Dibromochlorooxophosphorus(V)

[13550-31-7]

$Br_2P(O)Cl$

M 242.2

Synth. from $PCl_5 + PBr_3 + P_4O_{10}$. Solid. Fumes in moist air. d_4^{50} 2.45. Mp 31°. Bp 165°, Bp_{12} 49°.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 516 (*rev, bibl*)
King, S.T. *et al*, *Spectrochim. Acta, Part A*, 1970, **26**, 1481 (*ir, raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8**/III, 504, 1153 (*rev*)
Müller, A. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 219 (*ir, raman*)
Grossmann, G. *et al*, *Z. Chem.*, 1976, **16**, 362 (*O-17 nmr*)

IC-001769

Br_2ClP

Phosphorus bromide chloride (PBr_2Cl), 8Cl

Phosphorous dibromide chloride, 9*Cl*.
Dibromochlorophosphine. *Dibromochlorophosphorus*(III)

[13550-32-8]

PBr_2Cl

M 226.2

Obt. only as mixt. with $PBrCl_2$. Formed by equilibration between PBr_3 and PCl_3. Fuming liq. Protonated by 'magic' acid. V. reactive to protic nucleophiles. Bp 98-99°.

▷ Pungent vapour.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 514 (*rev, bibl*)
Müller, A. *et al*, *J. Mol. Struct.*, 1968, **2**, 149 (*ir, raman*)
Varmuza, K. *et al*, *Monatsh. Chem.*, 1971, **104**, 1037 (*synth, mt*)
Jordan, A.D. *et al*, *J. Chem. Phys.*, 1972, **56**, 483 (*synth, P-31 nmr*)
Dillon, K.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 63 (*synth*)
Van de Griend, L.J. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 5958 (*synth, P-31 nmr*)
Leipert, T.K. *et al*, *J. Chem. Phys.*, 1975, **63**, 4177 (*synth, P-31 nmr*)
Gloede, J. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **480**, 142 (*synth, P-31 nmr*)

Vengel'nikova, V.N. *et al*, *Zh. Obshch. Khim.*, 1982, **52**, 1318; *J. Gen. Chem. USSR (Engl. Transl.)*, 1982, **52**, 1160 (*synth, P-31 nmr*)

IC-001770

$Br_2Cl_2Fe^{\ominus}$

Dibromodichloroferrate(*III*)(1−), 11Cl

[31107-65-0]

$[FeBr_2Cl_2]^{\ominus}$ (C_{2v})

M 286.5 (ion)

Tetrahedral. Pesticide.

Et_4N salt: [28145-88-2].
Synth. from Et_4NCl and anhydrous iron(*III*) halide in anhydrous EtOH. Cryst. (anhydrous EtOH).

Clausen, C.A. *et al*, *Inorg. Chem.*, 1970, **9**, 220 (*ir, mössbauer, synth*)
Bhavsar, G.P. *et al*, *J. Mol. Struct.*, 1973, **16**, 343 (*ir*)
Balt, S. *et al*, *Z. Naturforsch., B*, 1978, **33**, 745 (*synth, ion association*)

IC-001771

$Br_2Cl_2P^{\oplus}$

Dibromodichlorophosphonium

Dibromodichlorophosphorus(1+), 9Cl

[36487-47-5]

$[PBr_2Cl_2]^{\oplus}$

M 261.6 (ion)

Obt. only in presence of other bromochlorophosphonium salts. Characterised spectroscopically in soln. Synth. from $PCl_3 + Br_2$, or from $PBr_3 + Cl_2$ in oleum or FSO_3H.

[50807-51-7, 50807-57-3]

Finch, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1863 (*synth, raman*)
Grimmer, A.R., *Z. Anorg. Allg. Chem.*, 1973, **400**, 105 (*P-31 nmr*)
Dillon, K.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1591 (*synth, P-31 nmr*)
Dillon, K.B. *et al*, *Polyhedron*, 1983, **2**, 641 (*formn, P-31 nmr*)

IC-001772

Br_2Cl_2Si

Dibromodichlorosilane

Silicon bromide chloride ($SiBr_2Cl_2$). Silicon dibromide dichloride

[13465-75-3]

$SiBr_2Cl_2$ (C_{2v})

M 258.7

Colourless liq. d_4^{25} 2.172. Mp −45.5°. Bp 104°. Dec. in H_2O.

Hoefler, F., *Z. Naturforsch., A*, 1971, **26**, 547 (*ir*)
Hass, D. *et al*, *Z. Chem.*, 1975, **15**, 240 (*synth*)
Niemann, U. *et al*, *Z. Naturforsch., B*, 1975, **30**, 202 (*Si-29 nmr*)
Brauer, G., *Handbuch Prdp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 680 (*synth*)
Sladkov, I.B. *et al*, *Zh. Fiz. Khim.*, 1982, **56**, 1032.

IC-001773

Br_2Cl_2Sn

Dibromodichlorostannane

Tin bromide chloride ($SnBr_2Cl_2$). Tin dibromide dichloride

[13550-35-1]

$SnBr_2Cl_2$ (C_{2v})

M 349.4

Colourless liq. d^{15} 2.82. Mp −20°. Bp_{30} 65°. Dec. in H_2O.

Ceri, C. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 389, 2818 (*ir*)
Lyubinov, V.S. *et al*, *Zh. Fiz. Khim.*, 1972, **46**, 838.
Shult, D.E., *Diss. Abstr. Int., B*, 1977, **38**, 187.
Colton, R. *et al*, *Inorg. Chim. Acta*, 1982, **61**, 1 (*Sn-119 nmr*)

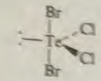
IC-001774

Br_2Cl_2Te

Dibromodichlorotellurium(*IV*)

Tellurium(IV) *bromide chloride* ($TeBr_2Cl_2$). *Tellurium dibromide dichloride*

[22968-35-0]



M 358.3

Various isomers known with Br in axial or equatorial positions. Synth. from $TeCl_2$ + liq. Br_2. Yellow cryst. melting to red liq. Stable in dry air. Dec. by H_2O to TeO_2. Mp 292°. Bp 415°.

Aynsley, E.E., *J. Chem. Soc.*, 1953, 3018 (*synth*)
Beattie, I.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 1747 (*synth, ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 11, 1978, **B3**, 50 (*bibl*)

IC-001775

$Br_2Cl_3Cu^{3\ominus}$

Dibromotrichlorocuprate(*II*)(3−), 10Cl

$[CuBr_2Cl_3]^{3\ominus}$

M 329.7 (ion)

Square-based pyramidal geometry at Cu.

N-(2-Ammoniumethyl)piperazinium(3+) salt: [73460-63-6].
Red-orange cryst. + $1H_2O$. Mp 205° dec. μ_{eff} = 1.85 μ_B

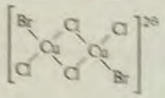
Antolini, L. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 1303 (*synth, ir, uv, magnetism*)

IC-001776

$Br_2Cl_4Cu_2^{2\ominus}$

Dibromodi-μ-chlorodichlorodicuprate(*II*)(2−), 10Cl

Dibromotetrachlorodicuprate(2−), 9Cl.
Bromodichlorocuprate(1−) dimer



M 428.7 (ion)

Presumed symmetrical dimer.

Bis-Ph_4P salt: [67577-05-3].
Deep purple cryst. Disproportionates on attempted recryst. Insol. EtOH.
Bis-Ph_4As salt: [53154-28-2].

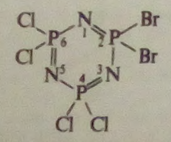
Chow, C. *et al*, *Inorg. Chem.*, 1975, **14**, 205 (*synth, magnetism*)
Estes, W.E. *et al*, *Inorg. Chem.*, 1978, **17**, 3657 (*synth, cor, uv, ir, magnetism*)

$Br_2Cl_4N_3P_3$ IC-001777

2,2-Dibromo-4,4,6,6-tetrachloro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 8CI

gem-*Dibromotetrachlorocyclotriphosphonitrile. 2,2-Dibromo-4,4,6,6-tetrachlorocyclotriphosphazene. 2,2-Dibromo-4,4,6,6-tetrachloro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2-Dibromo-4,4,6,6-tetrachloro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine*

[15969-71-8]



M 436.5

Not obt. free from non-gem isomer. Synth. from PCl_5 + NH_4Cl + PBr_3 in $C_2H_2Cl_4$. Solid. Mp 136.5°.

[25323-26-6]

Rice, R.G. *et al, J. Inorg. Nucl. Chem.*, 1958, **5**, 190 (*synth*)
Engelhardt, G. *et al, Z. Naturforsch., B*, 1966, **21**, 1231 (*P-31 nmr*)
Coxon, G.E. *et al, Inorg. Chim. Acta*, 1967, **1**, 381 (*synth*)

$Br_2Cl_4N_3P_3$ IC-001778

Dibromo-tetrachloro-2,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 8CI

vic-*Dibromotetrachlorocyclotriphosphonitrile. 2,4-Dibromo-2,4,6,6-tetrachlorocyclotriphosphazene. 2,4-Dibromo-2,4,6,6-tetrachloro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,4-Dibromo-2,4,6,6-tetrachloro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine*

[15964-99-5]

M 436.5

Unknown whether *cis* or *trans*. Synth. from PCl_5 + NH_4Br. Solid (C_6H_6). Mp 131° (129°).

Rice, R.G. *et al, J. Inorg. Nucl. Chem.*, 1958, **5**, 190 (*synth, ir*)
Engelhardt, G. *et al, Z. Naturforsch., B*, 1966, **21**, 1231 (*P-31 nmr*)
Coxon, G.E. *et al, Inorg. Chim. Acta*, 1967, **1**, 381 (*synth, ir*)
Coxon, G.E. *et al, J. Chem. Soc. A*, 1969, 358 (*ms*)

$Br_2Cl_{10}Ta_6^{4\oplus}$ IC-001779

Di-μ-bromodeca-μ-chlorohexatantalum(4+), 11CI

[94772-19-7]

$[Ta_6Cl_{10}Br_2]^{4\oplus}$

M 1600.0 (ion)

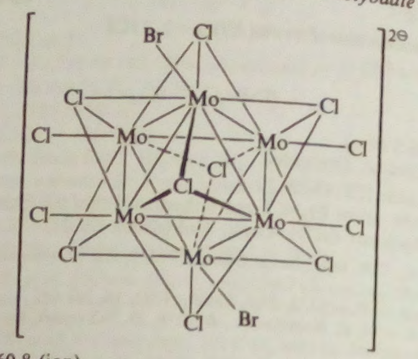
The positions of the Br atoms in the Ta_6X_{12} struct. are not known. Synth. by recryst. the $[Ta_6Br_6Cl_6]^{4\oplus}$ ion from HCl.

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1984, **517**, 185 (*synth*)

$Br_2Cl_{12}Mo_6^{2\ominus}$ IC-001780

Dibromoocta-μ₃-chlorotetrachlorohexamolybdate(2−), 11CI

Octakis(μ₃-chloro)dibromotetrachlorohexamolybdate



M 1160.8 (ion)

Br coordinated to two *trans*-Mo in $Mo_6Cl_8^{4\oplus}$ core cluster.

Bis-Ph_4As salt: [84220-71-3].
Cryst.

Schäfer, H. *et al, Z. Anorg. Allg. Chem.*, 1982, **491**, 275 (*cryst struct, synth*)

Br_2Co IC-001781

Cobalt(*II*) bromide ($CoBr_2$), 8CI

Cobalt dibromide

[7789-43-7]

$CoBr_2$

M 218.7

Dimorphous; has CdI_2 or $CdCl_2$ type structs. Commercially available. Green cryst. Sol. H_2O, Me_2CO, MeOH. Mp 678°. Paramagnetic.

▷ Toxic, irritant. GF9595000.

Dihydrate: [17670-82-5].
Purplish-blue solid. Prob. has octahedral polymeric struct. with 4 bridging Br.

Hexahydrate: [13762-12-4]. *Hexaaquacobalt(2+) bromide. Cobalt*(II) *bromide hexahydrate*
Red solid. Best considered as bromide salt of $[Co(OH_2)_6]^{2\oplus}$.

Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1379.
Wells, A.F., *Structural Inorg. Chem.*, 5th Ed., Oxford, 1984, 413 (*struct*)

Br_2Cr IC-001782

Chromium(*II*) bromide ($CrBr_2$)

Chromium dibromide. Chromous bromide

[10049-25-9]

$CrBr_2$

M 211.8

Distorted CdI_2 struct. in solid state. Dimeric in vapour state. Synth. from $CrBr_3$ and H_2 in presence of HBr; or by oxidation of Cr in a Br_2/H_2 stream at 800-900°. White cryst. solid. Rapidly oxidised in air. Blue in aq. soln. Sol. H_2O, EtOH. Mp 842°, 844°.

Hexahydrate: [18721-05-6]. *Hexaaquachromium(2+) dibromide. Chromium*(II) *bromide hexahydrate*
$Br_2CrH_{12}O_6$ M 319.8
Air-sensitive blue cryst.

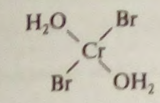
Bis-Py complex:
$C_{10}H_{10}Br_2CrN_2$ M 370.0
Green cryst. (EtOH). More stable than hydrate.

Fergusson, J.E., *Halogen Chem.*, Academic Press, London, 1967, 3, 229.
Inorg. Synth., 1967, **10**, 26 (*synth, hydrate*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1486 (*synth*)
Kovba, V.M., *Zh. Neorg. Khim.*, 1983, **28**, 2689; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 1525 (*ir, gas*)

$Br_2CrH_4O_2$ IC-001783

Diaquadibromochromium(*II*)

Chromium(II) *bromide dihydrate*



M 247.8

Square planar units obt. as complex with pyridinium bromide, $[CrBr_2(OH_2)_2].2[PyH]Br$ in which the expected formulation containing octahedral $[CrBr_4(OH_2)_2]^{2\ominus}$ units is not found. See Diaquatetrabromochromate(*II*)(2−), IC-002010. Interatomic distances: Cr—Br 257.9, Cr—O 203.8 pm.

Complex with pyridinium bromide (1:2): [50774-44-2].
Pyridinium diaquatetrabromochromate(II) (*incorr.*)
$C_{10}H_{16}Br_4CrN_2O_2$ M 567.8
Synth. from $CrBr_2$ + pyridinium bromide in HOAc. Light-green air-sensitive needles (HOAc).

Babar, M.A. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 27 (*deriv, synth, magnetism, uv*)
Ladd, M.F.C. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2351 (*deriv, cryst struct, synth*)

$Br_2CrH_{10}N_2O_2^{\oplus}$ IC-001784

Diamminediaquadibromochromium(*III*)(1+), 8CI

Dibromodiaquadiamminechromium(III)

$[CrBr_2(OH_2)_2(NH_3)_2]^{\oplus}$

M 281.8 (ion)

Octahedral cation. Hydrol. to Diamminetetraaquachromium(*III*)(3+), IC-017721.

all-trans-form

Bromide: Green cryst. + $1H_2O$. Sol. dil. aq. $HClO_4$.

[22941-60-2, 29560-95-0]

House, D.A., *Aust. J. Chem.*, 1969, **22**, 647 (*synth, uv, kinetics*)

Br_2CrO_2 IC-001785

Chromium(*VI*) bromide oxide ($CrBr_2O_2$)

Dibromodioxochromium, 9CI. Chromyl bromide. Chromyl dibromide

[14518-98-0]

CrO_2Br_2

M 243.8

Prepd. by reaction of CrO_2Cl_2 with excess liq. HBr at −60° to −80°. V. hygroscopic purple needles. Stable < −70°, dec. at r.t.

Zellner, H., *Monatsh. Chem.*, 1949, **80**, 317 (*synth*)
Krauss, H.L. *et al, Z. Naturforsch., B*, 1962, **17**, 1 (*synth, uv*)
Hope, E.G. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 1587 (*synth, ir*)

Br_2Cu IC-001786

Copper(*II*) bromide ($CuBr_2$), 11CI, 10CI, 9CI

Cupric bromide

[7789-45-9]

$CuBr_2$

M 223.3

Distorted CdI_2 struct. Wood preserver. Intensifier in photography. Black, deliquescent monoclinic cryst. V. sol. H_2O; sol. EtOH, Me_2CO; insol. C_6H_6, Et_2O. Mp 498°. Bp 900°.

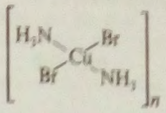
Di-NH_3 complex: see *Diamminedibromocopper*(II), *IC-001787*

Watt, G.W. *et al, J. Am. Chem. Soc.*, 1955, **77**, 2752 (*synth*)
Ramdall, S.P. *et al, J. Phys. Chem.*, 1959, **63**, 758 (*struct*)
Hougen, J.T. *et al, J. Chem. Phys.*, 1961, **34**, 1670 (*struct*)
Frost, D.C. *et al, Mol. Phys.*, 1972, **24**, 861 (*pe*)
Islam, N., *Indian J. Chem., Sect. A*, 1975, **13**, 1080 (*ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 977 (*synth*)
Iordanov, N. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 137 (*esr*)
Bastow, T.J. *et al, J. Mol. Struct.*, 1980, **58**, 305 (*nqr*)

$Br_2CuH_6N_2$ IC-001787

Diamminedibromocopper(*II*), 10CI, 9CI, 8CI

[21723-88-6]



M 257.4

Trans-square planar Cu has 2 additional axial interactions with Br from neighbouring molecules. Insol. Me_2CO.

α-form

Elongated rhombic cryst.

β-form

High pressure-form
Obt. from α-form under high pressure. Compressed tetragonal cryst.

[68499-84-3]

Hanic, F. *et al, Acta Crystallogr.*, 1958, **11**, 610; 1959, **12**, 739 (*cryst struct*)
Gazo, J., *Chem. Zvesti*, 1959, **13**, 3 (*synth*)
Tomlinson, A.A.G. *et al, J. Chem. Soc. A*, 1968, 2578 (*esr, ir, uv*)
Billing, D.E. *et al, J. Chem. Soc. A*, 1971, 2839 (*esr*)
Takeshi, A. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 974 (*magnetism*)
Papankova, B. *et al, Inorg. Chim. Acta*, 1982, **60**, 171 (*phys props*)

Br_2Dy IC-001788

Dysprosium bromide ($DyBr_3$)

Dysprosium dibromide

[83229-05-4]

$DyBr_2$

M 322.3

Has SrI_2 struct. Black solid.

Baernighausen, H., *Proc. Rare Earth Res. Conf., 12th, 1976*, 1976, 1, 404 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6**, 74 (*rev*)
Haschke, J.M. *et al, Handbook on the Physics and Chemistry of Rare Earths*, 1979, **4**, 119.
Friedt, J.M. *et al, Inorg. Chem.*, 1983, **22**, 2910 (*synth, mössbauer*)

Br_2Eu IC-001789

Europium bromide ($EuBr_2$)
Europium dibromide
[13780-48-8]

$EuBr_2$

M 311.7
Has $SrBr_2$ struct. Formed when $EuBr_3$ heated *in vacuo* >560°. Can be synth. from EuH_2 + Br_2 at 250-300°. White solid. Sol. H_2O. Mp 683° (677°). Bp 1880°, Subl. 1000° *in vacuo*. Paramagnetic, $\mu_{eff} = 7.93\mu_B$ (292K).

Klemm, W. *et al*, *Z. Anorg. Allg. Chem.*, 1939, **241**, 283 (*synth, magnetism*)
Spedding, F.H. *et al*, *Metall. Rev.*, 1960, **5**, 297.
Rossmanith, K., *Monatsh. Chem.*, 1966, **97**, 863 (*synth*)
Haschke, J.M., *J. Phys. Chem.*, 1970, **74**, 1806 (*synth, props*)
Haschke, J.M., *J. Chem. Thermodyn.*, 1973, **5**, 283 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6**, 66 (*rev*)
Sanchez, J.P. *et al*, *Inorg. Chem.*, 1985, **24**, 408 (*struct, mössbauer*)
Lyle, S.J. *et al*, *J. Less-Common Met.*, 1985, **106**, 109 (*synth*)
Golovanova, A.I. *et al*, *Zh. Neorg. Khim.*, 1985, **30**, 566; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1985, **30**, 330 (*synth*)

Br_2FOP IC-001790

Phosphoryl bromide fluoride ($POBr_2F$), 9CI, 8CI
Dibromofluorophosphine oxide.
Dibromofluorooxophosphorus(V)
[14014-19-8]

$Br_2P(O)F$

M 225.7
Synth. from $POBr_3$ + SbF_3. Liq. which fumes in moist air. Mp −117.2°. Bp 110.1°. ΔH_f (g) −682 kJ mol^{-1}.
▷ Dec. violently by H_2O.

Booth, H.S. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 3120 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 510 (*rev, bibl*)
Müller, A. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1967, **71**, 571 (*ir, raman*)
Müller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **350**, 246 (*ir, raman, F-19 nmr, P-31 nmr*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 455, 1153 (*rev*)
Binnewies, M. *et al*, *Thermochim. Acta*, 1986, **103**, 401 (*ms*)

Br_2FP IC-001791

Phosphorus bromide fluoride (PBr_2F), 8CI
Phosphorous dibromide fluoride, 9CI.
Dibromofluorophosphine. Dibromofluorophosphorus(III)
[15597-39-4]

PBr_2F

M 209.7
Reactive liq. which slowly disproportionates. May be distilled at atmos. press. d^0 2.181. Mp −115°. Bp 78.4°.

Booth, H.S. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 2934 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 509 (*rev, bibl*)
Müller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **350**, 256 (*ir, raman, F-19 nmr, P-31 nmr*)
Müller, A. *et al*, *Z. Naturforsch., B*, 1968, **23**, 588 (*ir, raman*)

Br_2FPS IC-001792

Thiophosphoryl bromide fluoride ($PSBr_2F$), 9CI, 8CI
Dibromofluorophosphine sulfide.
Dibromofluorothioxophosphorus(V)
[13706-10-0]

$Br_2P(S)F$

M 241.8
Interatomic distances (vap.): P═S 187, P—F 150, P—Br 218 pm; angle: BrPBr 100°. Synth. from $PSBr_3$ + SbF_3. Fuming liq. d^0 2.39. Mp −75°. Bp 125-125.5°.
▷ XN2980000.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 601 (*rev, bibl*)
Roesky, H.W., *Chem. Ber.*, 1967, **100**, 1447 (*synth, F-19 nmr, P-31 nmr*)
Müller, A. *et al*, *Z. Phys. Chem.* (*Frankfurt am Main*), 1967, **55**, 218 (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 534, 1153 (*rev*)
Müller, A. *et al*, *Spectrochim. Acta, Part A*, 1973, **29**, 219 (*ir, raman*)
Elbel, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1762 (*pe*)
Binnewies, M. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **552**, 147 (*synth, ms, reactions*)

Br_2FTl IC-001793

Thallium(*III*) bromide fluoride ($TlBr_2F$)

$TlBr_2F$

M 383.1
Synth. from Br_2 + TlF soln. in HF. Dec. by H_2O, sl. hygroscopic, stable *in vacuo*.
▷ Toxic.

Pascal, P., *Nouveau Traité de Chimie Minérale*, Masson, 1961, 6, 948 (*synth, prop*)

Br_2F_3Mo IC-001794

Molybdenum(*V*) bromide fluoride ($MoBr_2F_3$), 9CI
Molybdenum dibromide trifluoride
[42075-89-8]

$MoBr_2F_3$

M 312.7
Prepd. from MoF_3 and Br_2 at 100-130°. In vacuum, dec. to $MoBr_3$, MoF_5 and Br_2 at 140-150°.

Khaldoyanidi, K.A. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1973, 142; *CA*, **79**, 12985u (*synth*)

Br_2F_3P IC-001795

Phosphorus bromide fluoride (PBr_2F_3)
Dibromotrifluorophosphorane, 9CI.
Dibromotrifluorophosphorus(V)
[13445-58-4]

PBr_2F_3

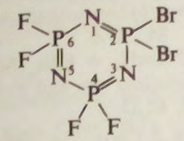
M 247.7
Tbp struct. with eq. Br atoms; fluorines in both axial and equatorial positions at −120°, but identical at r.t. Synth. from PF_3 + Br_2. At low temps, an unstable (dec. at −15°) molecular liq. Rapidly dec. at amb. temp. in poorly polar solvs. giving PBr_3, Br_2, PF_5.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 510 (*rev, bibl*)
Mahler, W. *et al*, *Inorg. Chem.*, 1965, **4**, 1520 (*F-19 nmr, struct*)

Wicker, W. *et al*, *Z. Naturforsch., B*, 1966, **21**, 1103 (*P-31 nmr, struct*)
Salthouse, J.A. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 1069 (*ir, struct*)
Dhamelincourt, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1970, **271**, 124 (*raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 449 (*rev*)
Vega, A.J. *et al*, *J. Magn. Reson.*, 1980, **37**, 107 (*synth, F-19 nmr*)

$Br_3F_4N_3P_3$ IC-001796

2,2-Dibromo-4,4,6,6-tetrafluoro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 8CI
1,3,5,2,4,6-triazatriphosphonitrile. 2,2-Dibromo-gem-Dibromotetrafluorocyclotriphosphonitrile. 2,2-Dibromo-4,4,6,6-tetrafluorocyclotriphosphazene. 2,2-Dibromo-4,4,6,6-tetrafluoro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2-Dibromo-4,4,6,6-tetrafluoro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine
[17022-76-3]

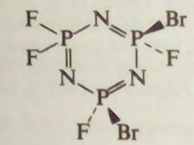


M 370.7
Synth. from $P_3N_3Br_6$ + AgF or KSO_2F in $PhNO_2$. Phys. props. not descr.

Steger, E. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1812 (*synth, ir*)
Clare, P. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 467 (*ir, ms*)

$Br_2F_4N_3P_3$ IC-001797

2,4-Dibromo-2,4,6,6-tetrafluoro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 9CI, 8CI
vic-Dibromotetrafluorocyclotriphosphonitrile. 2,4-Dibromo-2,4,6,6-tetrafluorocyclotriphosphazene. 2,4-Dibromo-2,4,6,6-tetrafluoro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,4-Dibromo-2,4,6,6-tetrafluoro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine
[29871-63-4]



cis-form

M 370.7
Synth. from $P_3N_3F_4(NMe_2)_2$ + HBr → *cis:trans* 55:45 mixt. Readily hydrol. Bp 151°.
cis-form [38589-72-9]
Isol. by gc.
trans-form [38589-73-0]
Isol. by gc.

Clare, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 2374 (*synth, F-19 nmr*)
Inorg. Synth., 1978, **18**, 194 (*synth, gc, F-19 nmr, ir*)
Clare, P. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 467, 477 (*ms*)
Clare, P. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 883 (*ir, raman*)

$Br_2F_4O_2Te$ IC-001798

Tellurium(*VI*) fluoride hypobromite ($TeF_4(BrO)_2$)
Tellurium tetrafluoride bis(hypobromite)
[79982-48-2]

$(BrO)_2TeF_4$

M 395.4
Synth. from $(ClO)_2TlF_4$ + Br_2. Moisture- and light-sensitive, thermally unstable.
cis-form
Red liq. Mp −31.5°. Dec. at 0°.
trans-form
Low-melting solid. Mp 23°.

Poetter, B. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1981, **20**, 1036 (*synth, F-19 nmr*)

$Br_2F_{12}FeP_4$ IC-001799

Dibromotetrakis(phosphorous trifluoride)iron(*II*), 9CI
Dibromotetrakis(trifluorophosphine)iron(II)
[37410-25-6]

$FeBr_2(PF_3)_4$

M 567.5
cis-Octahedral at Fe. Synth. from $Fe(PF_3)_5$ + Br_2. Orange-red, volatile. $Subl._{0.001}$ 20°. Dec. at 65°. $^1J_{PF}$ 1355 Hz.

Kruck, T., *Angew. Chem., Int. Ed. Engl.*, 1967, **6**, 53 (*rev*)
Kruck, T. *et al*, *Z. Naturforsch., B*, 1972, **27**, 344 (*synth, ir, nmr, mössbauer*)
Nixon, N.F., *Adv. Inorg. Chem. Radiochem.*, 1985, **29**, 41 (*rev*)

Br_2Fe IC-001800

Iron(*II*) bromide ($FeBr_2$)
Ferrous bromide
[7789-46-0]

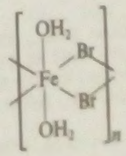
$FeBr_2$

M 215.6
Has CdI_2 struct. Synth. by action of (1) Br_2 vapour on Fe metal (2) HBr(g) on Fe metal. Starting material for iron(*II*) compds. Catalyst precursor. Polym. catalyst. Deliquescent yellow or brown cryst. V. sol. H_2O; sol. EtOH, Et_2O, MeCN. Mp 684° dec. Bp 967° extrap. $\mu_{eff} = 5.7\mu_B$ (295K).

Dihydrate: see *Diaquadibromoiron*(II), *IC-001801*
Tetrahydrate: see *Tetraaquadibromoiron*(II), *IC-001802*
Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, **II**, 1332 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, **B1**, 321 (*rev, bibl*)
Kühnl, E., *Z. Anorg. Allg. Chem.*, 1962, **317**, 84 (*synth*)
Colton, R. *et al*, *Halides of the First Row Transition Metals*, Wiley, N.Y., 1969 (*rev, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1642 (*synth*)

$Br_2FeH_4O_2$ IC-001801

Diaquadibromoiron(*II*)
Iron(II) *bromide dihydrate. Ferrous bromide dihydrate*
[20049-65-4]



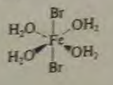
M 251.6
Polymeric chain struct. with approx. octahedral Fe. Obt. by recryst. of $FeBr_2$ from H_2O above 89°. Off-white solid.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, B1, 325 (rev, bibl)
Burbridge, C.D. *et al, J. Chem. Soc. A*, 1968, 1410 (*spectra, mössbauer, synth*)

IC-001802

$Br_2FeH_4O_4$

Tetraquadibromoiron(*II*)
Iron(II) *bromide tetrahydrate. Ferrous bromide tetrahydrate*



M 287.7
Octahedral.
trans-form [20049-61-0]
Obt. by recryst. of $FeBr_2$ from H_2O between 49-83°. Green-blue cryst.
Dihydrate: [13463-12-2]. *Iron*(II) *bromide hexahydrate*
Polym. catalyst. Deliquescent blue-green cryst., turns yellow-brown on exp. to air. Sol. H_2O, EtOH.
Pentahydrate: Iron(II) *bromide nonahydrate*
Obt. by recryst. of $FeBr_2$ from H_2O < −29.3°.
[20993-34-4, 20993-36-6]

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, B1, 325 (rev, bibl)
Burbridge, C.D. *et al, J. Chem. Soc. A*, 1968, 1410 (*mössbauer, synth, deriv*)

IC-001803

$Br_2FeN_2O_2^{\ominus}$

Dibromodinitrosylferrate(1−)
[24436-85-9]

$[Fe(NO)_2Br_2]^{\ominus}$ (C_{2v})

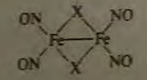
M 275.6 (ion)
Paramagnetic.

Schmidt, J., *Transition Met. Chem.*, 1976, **1**, 256 (*synth, esr*)
Glidewell, C. *et al, Polyhedron*, 1988, **7**, 1371 (*synth, esr*)

IC-001804

$Br_2Fe_2N_2O_4$

Di-μ-bromotetranitrosyldiiron, 9CI
Di-μ-bromobis(dinitrosyliron(I))
[15696-30-7]



X = Br

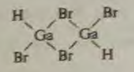
M 391.5
Black cryst. Subl.$_{1.9}$ 90°
Monomer: Bromodinitrosyliron
$BrFeN_2O_2$ M 195.7
Unknown.
[52394-43-1]

Soling, H. *et al, Acta Chem. Scand.*, 1957, **11**, 1534 (*synth*)
Beck, W. *et al, Chem. Ber.*, 1965, **98**, 2857 (*ir*)
Jones, R.F., *Diss. Abstr. Int., B*, 1972, **33**, 2516 (*use*)
Birchall, T. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2521 (*ir, mössbauer*)
Schmidt, J., *Transition Met. Chem.*, 1976, **1**, 256 (*reactions*)

Br_2GaH

IC-001805

Dibromogallane
Dibromogallium hydride. Gallium dibromide hydride
[13886-66-3]



dimer

M 230.5
Probable struct. shown.
Dimer: Tetrabromodigallane. Di-μ-bromodibromodihydrodigallium
$Br_4Ga_2H_2$ M 461.0
Synth. from $GaBr_3$ + Me_2SiH. Colourless air- and moisture-sensitive cryst. Mp −5°.
NMe$_3$ *complex (monomeric):* [17112-57-1].
Dibromohydro(trimethylamine)gallium
$C_3H_{10}Br_2GaN$ M 289.6
Synth. from Me_3NGaH_3 + HBr, $[Me_3NH]Br$, or Me_3NGaBr_3. Colourless air- and moisture-sensitive cryst. (C_6H_6). Sol. Et_2O.

Greenwood, N.N. *et al, J. Chem. Soc.*, 1965, 3426 (*synth, ir, pmr*)
Schmidbaur, H. *et al, Chem. Ber.*, 1967, **100**, 1129 (*synth, reactions*)

IC-001806

Br_2Ge

Germanium(*II*) bromide ($GeBr_2$), 9CI
Germanium dibromide
[24415-00-7]

$GeBr_2$

M 232.4
Polymeric. The monomer has been observed in the gas phase. Synth. from $GeBr_4$ + Ge. Cryst. Disproportionates to $GeBr_4$ and Ge at 150°. Hydrol. to $Ge(OH)_2$. Mp 143-144°.

Brewer, F.M. *et al, J. Phys. Chem.*, 1927, **31**, 1526 (*synth*)
Curtis, M.D. *et al, Inorg. Chem.*, 1972, **11**, 431 (*synth*)
Rouse, R.C. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1977, **145**, 161 (*cryst struct*)
Shultz, G. *et al, J. Mol. Struct.*, 1982, **82**, 107 (*struct*)
Van der Kerk, S.M., *Polyhedron*, 1983, **2**, 509 (*synth, ms*)

IC-001807

Br_2GeH_2

Dibromogermane, 9CI
[13769-36-3]

GeH_2Br_2

M 234.4
Synth. by direct reaction of Br_2 with GeH_4. Liq. d_4^0 2.80. Mp −15°. Bp 89°.

Dennis, L.M. *et al, J. Am. Chem. Soc.*, 1929, **51**, 2321 (*synth*)
Ebsworth, E.A.V. *et al, J. Mol. Spectrosc.*, 1964, **12**, 299 (*pmr*)
Beach, A.L. *et al, Can. J. Chem.*, 1966, **46**, 793 (*ir*)
Drake, J.E. *et al, J. Chem. Soc. A*, 1969, 2114 (*ir, raman*)
Beagley, B. *et al, J. Mol. Struct.*, 1973, **18**, 335 (*struct*)
Inorg. Synth., 1974, **15**, 157 (*synth*)

IC-001808

Br_2HN

Bromimide, 11CI, 10CI, 9CI
Dibromoamine
[14519-03-0]

Br_2NH

M 174.8
Synth. from NH_3 + Br_2 in Et_2O soln. Stable at −70° in Et_2O as a yellow soln. with irritating smell. λ_{max} 232 nm.

Inorg. Synth., 1939, **1**, 62 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 244.
Soulard, M. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 2300 (*anal, equilibria in soln*)

IC-001809

Br_2HZr_2

Zirconium bromide hydride (Zr_2Br_2H), 11CI
Dizirconium dibromide hydride
[60967-29-5]

HZr_2Br_2

M 343.2
The struct. is a distorted version of that of ZrBrH in which the hydride lies in zig-zag chains of distorted tetrahedra. Synth. by heating ZrBr in H_2. Bronze solid.
Deutero compd.: [105500-76-3]. *Dizirconium dibromide deuteride*
Br_2DZr_2 M 344.2
Bronze solid. Isomorphous with corresp. hydride.

Corbett, J.D. *et al, Inorg. Chem.*, 1983, **22**, 3194 (*pe*)
Marek, H.S. *et al, J. Less-Common Met.*, 1983, **89**, 243 (*synth, cryst struct, deuteride*)
Wijeyesekera, S.D. *et al, Inorg. Chem.*, 1986, **25**, 4709 (*cryst struct, deuteride*)

IC-001810

Br_2H_2Si

Dibromosilane
Silicon bromide hydride ($SiBr_2H_2$). *Silicon dibromide dihydride*
[13768-94-0]

SiH_2Br_2 (C_{2v})

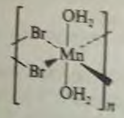
M 189.9
Colourless liq. d^0 2.17. Mp −70.1°. Bp 66°. Dec. in H_2O, alkali.
▷ Inflammable.

Egorochkin, A.N. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1971, 776 (*ir*)
Crudock, S. *et al, Trans. Faraday Soc.*, 1971, **67**, 3425 (*pe*)
Voronkov, M.G. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **232**, 817.
Belyi, A.P. *et al, Zh. Prikl. Khim. (Leningrad)*, 1978, **51**, 1407 (*synth*)

IC-001811

$Br_2H_4MnO_2$

Diaquadibromomanganese, 8CI
Manganese(II) *bromide* ($MnBr_2$) *dihydrate*
[13782-29-1]



M 250.7
Octahedral Mn in polymeric chain struct. Prepd. by evaporation of sat. aq. $MnBr_2$ at *ca.* 65°. Cryst. Isostructural with $MnCl_2.2H_2O$. Forms monohydrate at 70-137°.

Lawson, K.E., *J. Chem. Phys.*, 1966, **44**, 4159 (*synth, str*)
Morosin, B., *J. Chem. Phys.*, 1967, **47**, 417 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, C5, 284; 1983, C10, 47 (rev, bibl, str-str)

IC-001812

$Br_2H_4O_2Zn$

Diaquadibromozinc
Zinc bromide dihydrate. Hexaaquazinc(2+) *hexabromodizincate*(2−)
[18921-13-6]

$ZnBr_2.2H_2O$

M 261.2
The cryst. struct. is predicted to consist of $[Zn(OH_2)_6]^{2\oplus}$, and $[Zn_2Br_6]^{2\ominus}$ units. Cryst. V. sol. H_2O; sol EtOH; less sol. Et_2O. Mp 37°. Loses water on heating (100-245°). Isostructural with $[MgBr_2.2ZnBr_2.6H_2O]$.

Dietz, R.Z., *Z. Anorg. Allg. Chem.*, 1899, **20**, 247 (*synth*)
Brehler, B., *Fortschr. Mineral.*, 1961, **39**, 338 (*partial struct*)
Asker, W.J. *et al, Aust. J. Chem.*, 1972, **25**, 2301 (*ngr*)
Nirsha, B.M. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 931 (*thermal anal*)
Duhlev, R. *et al, Rev. Chim. Minér.*, 1986, **23**, 116.

IC-001813

$Br_2H_6HgN_2$

Diamminedibromomercury(*II*)
Mercuric bromide diammoniate. Diamminemercury dibromide
[21827-81-6]

$HgBr_2(NH_3)_2$

M 394.4
Polymeric struct. with bridging bromide and distorted octahedral Hg. White cryst. (NH_3). Insol. EtOH. Some dec. during removal of mother liquor after prep.

Gaudechon, H., *Comptr. Rend. Hebd. Seances Acad. Sci.*, 1909, **148**, 1703 (*synth*)
McGillavry, C.H. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1936, **94**, 231 (*cryst struct*)
Rüdorff, W. *et al, Z. Anorg. Allg. Chem.*, 1952, **270**, 145 (*cryst struct*)
Manolov, K.R., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 111 (*synth*)
Clark, R.J.H. *et al, J. Chem. Soc. A*, 1966, 1425 (*ir*)
Miles, M.G. *et al, Inorg. Chem.*, 1968, **7**, 1721 (*synth, ir, raman*)
Ebisuzaki, Y. *et al, J. Raman Spectrosc.*, 1982, **13**, 49 (*raman*)

IC-001814

$Br_2H_6N_2Zn$

Diamminedibromozinc(*II*)
Diamminezinc dibromide. Zinc(II) *bromide diammine*
[14591-92-5]

$(H_3N)_2ZnBr_2$

M 259.2
Cryst. Mp 235° dec.

MacGillavry, C.H. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1936, **94**, 249 (*cryst struct*)
Coates, G.E. *et al, J. Chem. Soc.*, 1964, 166 (*ir*)
Ablov, A.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 2288 (*heat of formn*)
Clark, R.J.H. *et al, J. Chem. Soc. A*, 1966, 1425 (*ir*)
Perchard, C. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 871 (*synth, ir, raman*)
Asker, W.J. *et al, Aust. J. Chem.*, 1972, **25**, 2301 (*synth, ngr, powder struct*)

IC-001815

$Br_2H_6N_4O_4Pt$

Diamminedibromodinitritoplatinum(*II*), 8Cl

Diamminedibromobis(nitrito-N)platinum(II), *9Cl*

[12011-06-2]

$Pt(NH_3)_2Br_2(NO_2)_2$

M 480.9

Much confusion and contradiction in earlier literature. Various isomers often not clearly specified, only the 'all *cis*' form is clearly established.

[19033-75-1, 19187-76-9, 56452-71-2]

Chernyaev, I.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 567 (*isom*)

Belova, V.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1966, **11**, 1435 (*magnetism*)

IC-001816

$Br_2H_8MnO_4$

Tetraaquadibromomanganese(*II*), 10Cl

Manganese(II) *bromide (MnBr$_2$) tetrahydrate*

[33572-60-0]

$MnBr_2(OH_2)_4$

M 286.8

Octahedral.

cis-form

Molecular. Prepared by evaporating sat. aq. $MnBr_2$ at r.t. Mp 87°. μ_{eff} = 5.93μ_B. Magnetic props. studied in detail.

trans-form

Metastable; detected in diffuse reflectance spectrum.

Zalkin, A. *et al, Inorg. Chem.*, 1964, **3**, 529 (*cis-form, struct*)

Oelkrug, D., *Naturwissenschaften*, 1968, **55**, 206 (*trans-form, uv*)

Schelleng, J.H. *et al, Phys. Rev.*, 1969, **185**, 728 (*cis-form, magnetism*)

Stein, R.L. *et al, J. Chem. Phys.*, 1970, **53**, 1031 (*cis-form, synth*)

Rupcheva, V.A. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 170 (*cis-form, thermal dec*)

Oelkrug, D. *et al, Ber. Bunsenges. Phys. Chem.*, 1972, **76**, 1088 (*trans-form, uv*)

Stein, R.L. *et al, Phys. Rev., B*, 1972, **6**, 1823 (*cis-form, synth, magnetism*)

Lawe, I.I. *et al, Phys. Rev., B*, 1972, **6**, 3262 (*cis-form, cryst struct*)

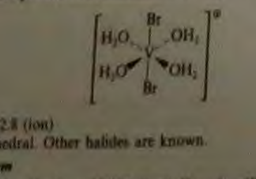
Sudarsanan, *Acta Crystallogr., Sect. B*, 1975, **31**, 2720 (*cis-form, cryst struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, **C5**, 275; 1983, **C10**, 47 (*rev, hibl, uv-vis*)

IC-001817

$Br_3H_6O_4V^{\oplus}$

Tetraaquadibromovanadium(*III*)(1+), 11Cl



M 282.8 (ion)

Octahedral. Other halides are known.

trans-form

Bromide, dihydrate: [56959-76-3]. *Vanadium*(III) *bromide hexahydrate*

$Br_3H_{12}O_4V$ M 398.7

Synth. by dissolving V in aq. HBr. Green cryst.

Paramagnetic, μ_{eff} = 2.85μ_B (297K), 2.70μ_B (86K).

Caesium bromide (1:2:3). [39710-53-7].

$Br_4Cs_2H_8O_4V$ M 788.3

Synth. by saturating an HBr soln. of $VBr_3.6H_2O$ and CsCl with HBr gas at 0°. Green cryst. Dehydrates to $Cs_2VCl_3.H_2O$.

Seifert, H.J. *et al, Inorg. Chem.*, 1966, **5**, 1822 (*synth*)

Podmore, L.P. *et al, Aust. J. Chem.*, 1972, **25**, 2521 (*synth, uv-vis, magnetism, nqr, ir*)

Donovan, W.F. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 894; 1976, 1741 (*cryst structs*)

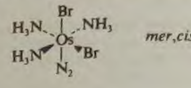
Bamberger, C.E. *et al, Inorg. Chim. Acta*, 1982, **57**, 161 (*thermal dec*)

Michalska-Fong, D. *et al, Spectrochim. Acta, Part A*, 1983, **39**, 835 (*ir, raman*)

IC-001818

$Br_2H_9N_5Os$

Triamminedibromo(dinitrogen)osmium(*II*)



mer,cis-form

M 429.1

mer-cis-form [73609-71-9]

Ir $\nu_{N\equiv N}$ 2010 cm^{-1}.

mer-trans-form [73557-96-7]

Ir $\nu_{N\equiv N}$ 2027, 2003 cm^{-1}.

Buhr, J.D. *et al, Inorg. Chem.*, 1980, **19**, 2425 (*synth, ir, uv*)

IC-001819

$Br_2H_{12}N_4Pt^{2\oplus}$

Tetraamminedibromoplatinum(*IV*)(2+), 8Cl

[41476-56-6]

$[PtBr_2(NH_3)_4]^{2\oplus}$

M 423.0 (ion)

Octahedral. Synth. by oxidation of $[Pt(NH_3)_4]^{2\oplus}$ $[PtBr_4]^{2\ominus}$

cis-form

Dibromide: [17125-87-0].

Dinitrate: [19066-47-8].

trans-form [16986-22-4]

More common isomer, esp. in double salts with Tetraammineplatinum(*II*)(2+), IC-019885.

Dibromide: [19066-45-6].

Orange-yellow needles (H_2O). Sol. H_2O.

Dinitrate: [19066-46-7].

Lemon-yellow plates. Sol. H_2O.

Tetraammineplatinum(II)*(2+)salt, perchlorate (1:1:4):* [76722-21-9].

Needles, dichroic: green-gold by reflection, red by transmission. Formulated as $[Pt(NH_3)_4][Pt(NH_3)_4Br_2][ClO_4]_4$.

▷ Potentially explosive.

Tetraammineplatinum(II) *(hydrogensulfate) (1:1:4):* [76687-78-0]. catena-*Tetra-ammine-μ-bromo-platinum*(II,IV) *tetrakis(hydrogensulfate)*

Needles, dichroic: green-gold by reflection, purple by transmission.

[16971-63-4, 19033-16-0, 19066-45-6, 84086-02-2, 87525-33-5]

Gmelin Handbook Inorg. Chem., Syst. No. 68, **D**, 501 (*synth*)

Gusev, A.I. *et al, Zh. Strukt. Khim.*, 1970, **11**, 62 (*struct*)

Layek, D. *et al, Z. Naturforsch., B*, 1981, **36**, 83 (*synth, raman*)

Tanaka, M. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 2793 (*synth, struct*)

Clark, R.J.H. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 2505 (*synth, struct, ir, raman, double salts*)

IC-001820

$Br_2H_{12}N_4Ru^{\oplus}$

Tetraamminedibromoruthenium(*III*)(1+), 9Cl

$[Ru(NH_3)_4Br_2]^{\oplus}$

M 329.0 (ion)

Approx. octahedral. Aq. anation reactions proceed *via* initial hydrolysis step. Sol. H_2O.

cis-form [42281-09-4]

Much more labile towards aquation than *trans*-form. Synth. from $[Ru(NH_3)_4(C_2O_4)]^{\oplus}$ and aq. HBr.

Bromide:

$Br_3H_{12}N_4Ru$ M 408.9

Dark red-brown solid. Thermal dec. → $[Ru(NH_3)_3Br_3]$. μ_{eff} = 1.93μ_B.

trans-form [43111-99-5]

Synth. by oxidation of $[Ru(NH_3)_4(SO_2)Br]Br$ with Br_2/HBr.

Chloride:

$Br_2ClH_{12}N_4Ru$ M 364.4

Bromide: Violet-red solid. μ_{eff} = 2.02μ_B.

Tribromide(1−):

$Br_5H_{12}N_4Ru$ M 568.7

Gleu, K. *et al, Z. Anorg. Allg. Chem.*, 1938, **237**, 326; 1939, **237**, 350 (*synth, magnetism*)

Movius, W.G. *et al, J. Am. Chem. Soc.*, 1970, **92**, 2677 (*uv*)

Ohyoshi, A. *et al, Bull. Chem. Soc. Jpn.*, 1973, **46**, 2133; 1974, **47**, 841, 1414; 1975, **48**, 230 (*photoaquation, tga, dta, cis-form*)

Allen, A.D. *et al, Can. J. Chem.*, 1973, **51**, 92 (*uv, theory*)

Verdonck, E. *et al, Inorg. Chem.*, 1974, **13**, 762 (*uv, theory*)

Kobata, S. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 768 (*theory*)

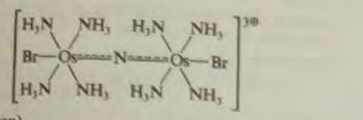
IC-001821

$Br_2H_{24}N_9Os_2^{3\oplus}$

Octaamminedibromo-μ-nitridodiosmium(*IV*)(3+)

μ-Nitridobis[tetraamminebromoosmium(IV)]

[65494-24-8]



M 690.4 (ion)

Complexes of the form $[Os_2N(NH_3)_8X_2]X_3$, (X = Cl,F,NCS,N_3,NO_3) are also known.

Tribromide: [128821-70-5].

Obt. by reaction of $K_2[OsBr_6]$ in liq. NH_3, followed by washing with EtOH. Tan coloured solid (dil. aq. HBr).

Ir ν_{N-H} 3440s, 3125s, ν_{Os-Br} 240br cm^{-1}.

[27119-87-1]

Watt, G.W. *et al, J. Inorg. Nucl. Chem.*, 1958, **6**, 246 (*synth*)

Griffith, W.P., *J. Chem. Soc.*, 1965, 3695 (*ir*)

Hewkin, D.J. *et al, J. Chem. Soc. A*, 1966, 472 (*ir*)

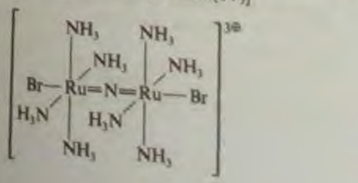
Cleare, M.J. *et al, J. Chem. Soc. A*, 1970, 1117 (*synth, ir*)

IC-001822

$Br_2H_{24}N_9Ru_2^{3\oplus}$

Octaamminedibromo-μ-nitridodiruthenium(*IV*)(3+), 8Cl

μ-Nitridobis[tetraamminebromoruthenium(IV)]



M 512.1 (ion)

Diamagnetic.

Tribromide: [27056-02-6].

Prepd. by treating $[Ru_2NCl_4(OH_2)_2]^{\oplus}$ with aq. NH_3, followed by aq. HBr. Orange salt. Ir ν_{Ru-N} 1039 cm^{-1}.

Cleare, M.J. *et al, J. Chem. Soc., Dalton Trans.*, 1970, 1117 (*synth, ir, raman*)

IC-001823

Br_4Hf

Hafnium(*II*) bromide ($HfBr_4$), 10Cl

Hafnium dibromide

[13782-95-1]

$HfBr_4$

M 338.2

Precise struct. unknown. Synth. by heating $HfBr_4$ and Hf to 450° or by disproportionation of $HfBr_3$. Blue-black solid which disproportionates above 400° to Hf and $HfBr_4$.

Larsen, E.M. *et al, J. Am. Chem. Soc.*, 1956, **78**, 5983 (*comkh*)

Marek, G.S. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1303 (*synth, struct*)

IC-001824

Br_2Hg

Mercury(*II*) bromide ($HgBr_2$)

Mercuric bromide

[7789-47-1]

$HgBr_2$

M 360.3

Struct. may be descr. as containing linear Br—Hg—Br molecules or as v. distorted CdI_2 struct. Linear molecule in the vapour. Used in thermog. materials. Sublimeable colourless cryst.; yellow liq. Sol. EtOH (30 g per 100 cm^3 at 25°), MeOH, HCl, HBr, alkali bromide solns.; spar. sol. H_2O (0.6 g per 100 cm^3 at 25°), $CHCl_3$. Mp 238°. Bp 318°.

▷ OV7415000.

Coates, G.E. *et al, J. Chem. Soc.*, 1964, 166 (*liar ir*)

Gmelin Handbook Inorg. Chem., Syst. No. 34, 1967, **B2**, 732

Beattie, I.R. *et al, J. Chem. Soc. A*, 1970, 2433 (*raman, gas*)

Wendlandt, W.W., *Thermochim. Acta*, 1974, **10**, 101 (*thermal anal*)

Glockling, F. *et al, Inorg. Chim. Acta*, 1976, **19**, 267 (*ms*)

Givan, A. *et al, J. Chem. Phys.*, 1976, **64**, 1967 (*matrix, ir, raman*)

Adams, D.M. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 776 (*ir, raman of cryst*)

Wulfsberg, G. *et al, Ber. Bunsenges. Phys. Chem.*, 1980, **84**, 474 (*nqr*)

Belevantiev, V.I. *et al, Koord. Khim.*, 1980, **6**, 1000 (*uv in aq and other solns*)

Lee, E.R.F. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1981, **22**, 247 (*pe*)

Albright, M.J. *et al, J. Organomet. Chem.*, 1983, **259**, 37 (*Hg-199 nmr, soln*)

Deyanov, R.Z. *et al, Zh. Strukt. Khim.*, 1985, **26**, 58 (*ed*)

Konovalov, L. *et al, J. Coord. Chem.*, 1986, **14**, 201 (*ir*)

Adams, D.M. *et al, J. Phys. C*, 1987, **20**, 6103 (*phase trans, raman*)

Masucci, J.A. *et al, Org. Mass Spectrom.*, 1987, **22**, 233 (*ms*)

Savas, M.M. *et al, Inorg. Chem.*, 1988, **27**, 658 (*uv, gas*)

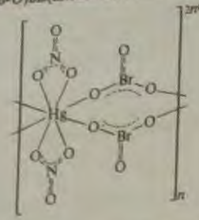
Hormes, J. *et al, Phys. Scr.*, 1988, **37**, 694 (*vacuum uv*)

Korshun, M.N. *et al, Gig. Sanit.*, 1989, **69**; *C.A.* **110**, 149419 (*toxic*)

Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2195.

$Br_2HgN_2O_{12}^{2\ominus}$ IC-001825

Bis(bromato-*O*)bis(nitrato-*O*,*O'*)mercurate(2−)



M 580.4 (ion)
Polymeric chain struct. with severely distorted sq. antiprismatic Hg.

Di-K salt: [80440-81-9].
From $KBrO_3$ and $Hg(NO_3)_2$ in 3*M* HNO_3. Cryst.

Aurivillius, K. *et al*, *Acta Chem. Scand., Ser. A*, 1981, **35**, 537 (*synth, cryst struct*)

Br_2HgO_6 IC-001826

Mercury(*II*) bromate ($Hg(BrO_3)_2$)

$Hg(BrO_3)_2$

M 456.3
Obt. by dehydration of dihydrate at 90° over P_2O_5. Solid. Sl. dec. at 140°.

▷ Explosive dec. at 155-160°.

Dihydrate: [26522-91-8]. *Diaquabis(bromato-O)mercury*
Synth. from $Hg(NO_3)_2$ and $NaBrO_3$ in 3*M* HNO_3. Cryst. (H_2O). Spar. sol. H_2O (0.15g per 100 cm^3 cold). Mp 130-140° dec. Contains 8-coord. Hg in solid state with coordn. by $2H_2O$, 2 bidentate $BrO_3^\ominus$ and 2 monodentate $BrO_3^\ominus$. Isomorphous with Cd analogue.

Smith, G.F., *J. Am. Chem. Soc.*, 1924, **46**, 1577 (*synth, anhydrous salt*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1967, **B2**, 812 (*rev, bibl*)
Aurivillius, K. *et al*, *Acta Chem. Scand., Ser. A*, 1981, **35**, 537 (*synth, cryst struct, dihydrate*)
Alexova, A. *et al*, *Collect. Czech. Chem. Commun.*, 1988, **53**, 1156 (*synth*)

Br_2Hg_4 IC-001827

Mercury(*I*) bromide (Hg_2Br_2)

Mercurous bromide

[15385-58-7]

Br—Hg—Hg—Br

M 560.9
Struct. comprises linear molecule (tetragonal) with 4 additional long Hg—Br contacts. Has application in accousto-optical devices. Light-sensitive white cryst. Pract. insol. H_2O (4×10^{-6} g per 100 cm^3 at 25°). Subl. 345° Dec. to $HgBr_2$ and Hg. Ferroelec. phase forms at 143 K. Exhibits orange fluorescence and becomes black under uv light. K_{sp} 6.40×10^{-23}

Monomer:
BrHg M 280.4
Has no separate existence.

Belov, N. *et al*, *Trud Kryst. Akad. Nauk. SSSR*, 1947, **87**, 819 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1967, **B3**, 722

Stammreich, H. *et al*, *J. Mol. Struct.*, 1967, **1**, 55 (*raman*)
Dorm, E., *Chem. Comm. Univ. Stockholm*, 1970, 3 (*cryst struct*)
Osaka, T. *et al*, *J. Chem. Phys.*, 1971, **54**, 863 (*far ir*)
Osaka, T. *et al*, *Opt. Spektrosk.*, 1974, **37**, 95 (*raman*)
Barta, C. *et al*, *Opt. Commun.*, 1976, **17**, 425 (*uv*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1052 (*synth*)
Barta, C. *et al*, *Abh. Akad. Wiss. DDR, Abh. Math. Naturwiss., Tech.*, 1977, **5**, 261 (*opt, electro-opt props*)
Bryker, Z. *et al*, *Cryst. Res. Technol.*, 1982, **17**, 425 (*uv*)
Konovalev, L. *et al*, *J. Coord. Chem.*, 1986, **14**, 201 (*ir*)
Zadokhin, B.S. *et al*, *Fiz. Tverd. Tela (Leningrad)*, 1987, **29**, 187 (*phase trans*)
McCarthy, K.A. *et al*, *Opt. Commun.*, 1987, **64**, 157 (*opt rotn of cryst*)
Kaplyanskii, A.K. *et al*, *Indian J. Pure Appl. Phys.*, 1988, **26**, 252 (*phase trans, raman*)
Oppermann, H. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **568**, 187 (*thermal anal*)

$Br_2Hg_2O_6$ IC-001828

Mercury(*I*) bromate

Bis(bromato-O)dimercury. Mercurous bromate

[13465-33-3]

$O_2BrOHgHgOBrO_2$

M 656.9
Linear, 2-coord. Hg. Synth. from $Hg_2(NO_3)_2$ and $KBrO_3$ in dil. aq. acid. Colourless cryst, unstable to x-rays. With $H_2O \rightarrow Hg_2(BrO_3)_2.Hg_2O$.

Dorm, E. *et al*, *Acta Chem. Scand.*, 1967, **21**, 1661, 2834 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1967, **B2**, 811 (*rev, bibl*)
Adams, D.M. *et al*, *J. Raman Spectrosc.*, 1976, **5**, 63 (*raman*)
Alexová, A. *et al*, *Collect. Czech. Chem. Commun.*, 1988, **53**, 1156 (*synth*)

$Br_2Hg_3S_2$ IC-001829

Mercury(*II*) bromide sulfide ($Hg_3Br_2S_2$)

Trimercury dibromide disulfide

[12048-98-5]

$Hg_3Br_2S_2$

M 825.7
3 cryst. modifications: α- (low temp.-form), β- (high temp.-form) both orthorhombic, and γ-form which is metastable. Synth. from Hg_2Br_2 and S or $HgBr_2$ and HgS (at 450°). Yellow cryst., stable to air and to conc. HCl, but not $OH^\ominus$.

Jander, G. *et al*, *Z. Anorg. Allg. Chem.*, 1951, **264**, 57 (*synth*)
Takei, K., *Bull. Chem. Soc. Jpn.*, 1955, **28**, 408; 1976, **49**, 1425 (*synth, phototropy*)
Batsanov, S.S. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1961, 67.
Puff, H. *et al*, *Naturwissenschaften*, 1962, **49**, 299; 1966, **53**, 274 (*synth, cryst struct*)
Batsanov, S.S. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1973, **9**, 1098 (*synth, props*)

$Br_2Hg_3Se_2$ IC-001830

Mercury(*II*) bromide selenide ($Hg_3Br_2Se_2$)

Trimercury dibromide diselenide

[12233-92-0]

$Hg_3Br_2Se_2$

M 919.4

Struct. contains octahedral Hg (3Se and 3Br) and $SeHg_3$ pyramids. Synth. from HgSe and $HgBr_2$ or Hg_2Br_2 and Se. Yellow cryst., stable to H_2O and conc. HCl but not $OH^\ominus$.

Jander, G. *et al*, *Z. Anorg. Allg. Chem.*, 1951, **264**, 57 (*synth*)
Batsanov, S.S. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1961, 67 (*synth*)
Puff, H. *et al*, *Naturwissenschaften*, 1962, **49**, 299 (*synth, cryst struct*)
Batsanov, S.S. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1973, **9**, 1098 (*synth, props*)

$Br_2Hg_3Te_2$ IC-001831

Mercury(*II*) bromide telluride ($Hg_3Br_2Te_2$)

Trimercury dibromide ditelluride

[12233-93-1]

$Hg_3Br_2Te_2$

M 1016.7
Infinite struct. with octahedral Hg (3Te and 3Br) and $TeHg_3$ pyramids. Synth. from Hg_2Br_2 and Te. Yellow cryst., stable to H_2O and conc. HCl, but not $OH^\ominus$.

Batsanov, S.S. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1961, 67 (*synth*)
Puff, H. *et al*, *Naturwissenschaften*, 1962, **49**, 299, 464 (*synth, cryst struct*)
Khodadad, P. *et al*, *Ann. Chim. (Paris)*, 1965, **10**, 83 (*synth, cryst struct*)
Batsanov, S.S. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1973, **9**, 1098 (*synth, props*)
Dovgoshei, V.N. *et al*, *Ukr. Fiz. Zh. (Russ. Ed.)*, 1985, **30**, 1721 (*ir*)

$Br_2Hg_5O_4$ IC-001832

Mercury bromide oxide ($Hg_5Br_2O_4$)

Basic mercury bromide

$Hg_5O_4Br_2$

M 1226.7
Solid state struct. contains both distorted octahedral ($HgBr_2O_4$) and tetrahedral (HgO_4) environments. Chestnut coloured cryst.

Pelabon, H., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1925, **180**, 1500 (*synth*)
Lamure, *Bull. Soc. Chim. Fr.*, 1948, 1019 (*synth*)
Aurivillius, K., *Ark. Kemi.*, 1964, **23**, 469 (*cryst struct*)

$Br_2I^\ominus$ IC-001833

Dibromoiodate(*I*)(1−)

[14791-49-2]

$[Br—I—Br]^\ominus$

M 286.7 (ion)
Linear struct., may or may not be symmetrical depending on counter cation. Forms red salts. Dissociates in H_2O.

K salt: [50967-92-5].
Br_2IK M 325.8
Synth. from KNO_3, I_2 and HBr. Solid + $1H_2O$. Dec. on exposure to atmosphere.

Cs salt: [18278-82-5].
Br_2CsI M 419.6
Synth. from stoichiometric amounts of bromide and iodide in a satd. soln. of CsBr. Dark orange cryst. Linear unsymmetrical. I—Br 262, 278 pm. Dec. on melting.

Me_4N salt: [15801-99-7].
Synth. from Me_4NI and Br_2 in EtOH. Dark orange cryst. (EtOH). Mp 192°.

Tetrapropylammonium salt: Synth. from Pr_4NI and Br_2 in EtOH. Dark orange cryst. (EtOH). Mp 139-140°.

Wells, H.L. *et al*, *Am. J. Sci.*, 1892, **43**, 417 (*synth*)
Inorg. Synth., 1957, **5**, 167.
Carpenter, G.B., *Acta Crystallogr.*, 1966, **20**, 330 (*cryst struct*)
Maki, A.G. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 867 (*ir, raman*)
Hayward, G.C. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2389 (*ir, raman*)
Davies, J.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 1374 (*struct, Cs salt*)
Gabes, W. *et al*, *J. Mol. Struct.*, 1972, **14**, 267 (*struct*)
Coignac, J.P. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 1365 (*struct, ir, Cs salt*)
Riedel, E.F. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 701 (*mgn*)

$Br_2I^\oplus$ IC-001834

Dibromoiodine(1+)

[11078-77-6]

$[Br—I—Br]^\oplus$

M 286.7 (ion)
Bent ion. Red cation. Dissociates in H_2O.

Undecafluorodiantimonate: [56664-97-2].
$Br_2F_{11}ISb_2$ M 739.1
Complicated synth. from SbF_5 + IBr in SO_2, followed by addn. of SO_2ClF soln. Shiny dark needles. Mp 139°. Fluorosulfate and chlorosulfate complexes also known.

Yeats, P.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 209 (*synth*)
Wilson, W.W. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 665 (*synth*)
Birchall, T. *et al*, *Inorg. Chem.*, 1983, **22**, 1751 (*synth, cryst struct, $Sb_2F_{11}^\ominus$ salt*)
Zaidi, S.A. *et al*, *Bull. Soc. Chim. Fr.*, 1987, 441 (*synth*)

$Br_2I_2P_2$ IC-001835

Hypodiphosphorous dibromide diiodide, 10Cl

P,P-Dibromo-P',P'-diiododiphosphine. 1,1-Dibromo-2,2-diiododiphosphine. 1,1-Dibromo-2,2-diiododiphosphorus(III). 1,1-Dibromo-2,2-diiododiphosphane

[79988-19-5]

Br_2PPI_2

M 475.5
Obt. only in mixt. with symmetrical isomer, Hypodiphosphorous dibromide diiodide, IC-001836. Synth. from P_2I_4 + PBr_3.

Dillon, K.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1981, **17**, 201 (*synth, P-31 nmr*)

$Br_2I_2P_2$ IC-001836

Hypodiphosphorous dibromide diiodide, 10Cl

P,P'-Dibromo-P,P'-diiododiphosphine. 1,2-Dibromo-1,2-diiododiphosphine. 1,2-Dibromo-1,2-diiododiphosphorus(III). 1,2-Dibromo-1,2-diiododiphosphane

[79988-21-9]

BrIPPIBr

M 475.5
Obt. only as mixt. with isomer Hypodiphosphorous dibromide diiodide, IC-001835. Synth. from P_2I_4 + PBr_3.

Dillon, K.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1981, **17**, 201 (*synth, P-31 nmr*)

Br_2I_2Sn IC-001837

Dibromodiiodostannane

Tin bromide chloride ($SnBr_2Cl_2$). Tin dibromide diiodide

[13550-40-8]

$SnBr_2I_2$ (C_{2v})

M 532.3

Synth. by mixing $SnBr_4$ and SnI_4 in 1:1 ratio. Orange-red hexagonal plates. Sol. cold H_2O; dec. in H_2O < 80°. d^{25} 3.631. Mp 50°. Bp 225°.

Cerf, C. et al, Bull. Soc. Chim. Fr., 1964, 389, 2818 (ir)
Gaizer, F. et al, Acta Chim. (Budapest), 1973, 77, 385.
Colton, R. et al, Inorg. Chim. Acta, 1982, 61, 1 (Sn-119 nmr)

Br_2I_2Te IC-001838

Tellurium(*IV*) bromide iodide ($TeBr_2I_2$)

Tellurium dibromide diiodide. Dibromodiiodotellurium

$TeBr_2I_2$

M 541.2

Formed from $TeBr_2$ + I_2. Red solid, purple vapour. Mp 323°. Bp 420° dec.

Aynsley, E.E. et al, J. Chem. Soc., 1955, 2603 (synth)
Gmelin Handbook Inorg. Chem., Syst. No. 11, 1978, B3, 49 (rev)

$Br_2In^{\ominus}$ IC-001839

Dibromoindate(1−)

$[InBr_2]^{\ominus}$ (C_{2v})

M 274.6 (ion)

See also under Hexabromodiindate(2−), IC-002152.

Et_4N salt: [57650-22-3].

Synth. from C_2H_5In, HBr, and $[Et_4N]Br$ in C_6H_6/EtOH. Colourless moisture-sensitive cryst. Spar. sol. C_6H_6, Et_2O.

Habeeb, J.J. et al, J. Chem. Soc., Dalton Trans., 1976, 866 (synth, ir, raman)
Freeland, B.H. et al, Can. J. Chem., 1977, 55, 1527 (pe, esca)

Br_2Mg IC-001840

Magnesium bromide ($MgBr_2$), 8Cl

[7789-48-2]

$MgBr_2$

M 184.1

CdI_2 struct. Prepd. by reaction of magnesium metal with $[NH_4]Cl$ in liq. NH_3. White, hexagonal cryst., deliquescent. V. sol. H_2O (101.5 g per 100 cm^3 at 20°, 125.6 g per 100 cm^3 at 100°), sol. EtOH, MeOH. Mp 711°. ΔH_f° −524 kJ mol^{-1}; ΔG_f° −504 kJ mol^{-1}; S° 117 J K^{-1} mol^{-1}.

▷ Irritant.

Hexahydrate: [13446-53-2]. *Hexaaquamagnesium(2+) dibromide*

$Br_2H_{12}MgO_6$ M 292.2

Commercially available. Heat storage material used in conjunction with $CaCl_2.6H_2O$. Colourless, hygroscopic, monoclinic cryst.; dec. on heating with loss of H_2O and hydrol. V. sol. H_2O (316 g per 100 cm^3 H_2O at 0°); sol. Me_2CO, EtOH. Mp 172.4°. ΔH_f° −2410 kJ mol^{-1}; ΔG_f° −2056 kJ mol^{-1}; S° 397 J K^{-1} mol^{-1}.

Et_2O complex: [29858-07-9].

$C_4H_{10}Br_2MgO$ M 258.2

Commercially available reagent for conversion of aliphatic ethylene oxides and cyclohexene oxides to corresp. ketones. Mp > 300°.

▷ Flammable.

Ferraro, A. et al, Atti R. Accad. Naz. Lincei, Rend. Cl. Sci. Fis., Mat. Nat., 1929, 9, 1134 (cryst struct)
Balkov, V.I., Opt. Spektrosk., 1969, 27, 923; CA, 1970, 72, 72794 (ir)
Sorrell, C.A. et al, J. Chem. Eng. Data, 1974, 19, 307 (cryst struct, hexahydrate)
Ergin, Yu.V. et al, Zh. Strukt. Khim., 1974, 15, 391 (magnetism)
Hadenfeldt, C., Z. Naturforsch., B, 1975, 30, 165 (synth)
Heubel, P.H. et al, J. Solution Chem., 1979, 8, 283 (Mg-25 nmr)
McCormick, J.P. et al, J. Org. Chem., 1980, 45, 2566 (ether complex)
Anderson, A. et al, Spectrosc. Lett., 1981, 14, 603 (ir, raman)
Kimura, H. et al, Energi Shigen, 1985, 6, 528; CA, 104, 92081 (heat storage, hexahydrate)
Chase, M.W. et al, J. Phys. Chem. Ref. Data, 1985, 14, 477.
Halut-Desportes, S., Spectrochim. Acta, Part A, 1985, 41, 661 (ir, hexahydrate)
Naumann, R. et al, Therm. Anal., 1985, 92, 673 (thermal dec, hexahydrate)

Br_2Mn IC-001841

Manganese(*II*) bromide ($MnBr_2$)

Manganese dibromide

[13446-03-2]

$MnBr_2$

M 214.7

CdI_2 layer struct. Synth. from $MnCO_3$ and aq. HBr followed by dehydration at 100° and drying in HBr gas at 725°. Alternatively obt. from $Mn(OAc)_2.4H_2O$ and AcBr in C_6H_6. Commercially available. Pink hygroscopic solid. V. sol. H_2O. Mp 698° (695°). Does not obey Curie or Curie-Weiss law at normal temps. T_N 2.16K. μ_{eff} = 5.82μ_B (298K). Forms adducts with donor molecules.

Watt, G.W. et al, J. Am. Chem. Soc., 1955, 77, 2752 (synth)
Brewer, L. et al, Chem. Rev., 1963, 63, 111 (rep)
Hadley, W.B. et al, J. Chem. Phys., 1963, 39, 2205 (synth, magnetism)
Seifert, H.J. et al, Z. Anorg. Allg. Chem., 1972, 391, 302 (struct)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, C5, 264; 1983, C10, 45 (rev, bibl, ur-vis)

Br_2MoN IC-001842

Molybdenum(*V*) bromide nitride ($MoBr_2N$)

Molybdenum(V) nitridobromide ($MoNBr_2$)

[72142-91-7]

$MoBr_2N$

M 269.7

Incorrectly indexed in CA as MoBrN. Prepd. by thermolysis of $MoNBr_3$ *in vacuo* at 260°. Dark green hygroscopic powder. Stable below 420°. Ir indicates a Mo—N multiple bond.

Krueger, N. et al, Z. Naturforsch., B, 1979, 34, 1343 (synth, ir)

Br_2MoO_2 IC-001843

Molybdenum(*VI*) bromide oxide ($MoBr_2O_2$)

Molybdenum oxybromide (MoO_2Br_2).

Dibromodioxomolybdenum(VI)

[13595-98-7]

Br_2MoO_2

M 287.7

Prepd. by bromination of MoO_2 in the presence of activated charcoal or by reaction of $COBr_2$ with MoO_2. Red-brown flakes. Sol. H_2O.

Colton, R. et al, Aust. J. Chem., 1965, 18, 447 (synth)
Barraclough, C.G. et al, Aust. J. Chem., 1966, 19, 741 (ir, ms, struct)
Adams, D.M. et al, J. Chem. Soc. A, 1968, 2310 (ir, raman)
Oppermann, H., Z. Anorg. Allg. Chem., 1970, 379, 262 (thermodyn)
Singleton, D.L. et al, Inorg. Chem., 1972, 11, 1208 (mc)
Drobot, D.V. et al, Russ. J. Inorg. Chem. (Engl. Transl.), 1975, 20, 2108 (synth)
Levason, W. et al, J. Chem. Soc., Dalton Trans., 1982, 2009 (ir, ue)
Parkinson, M.J. et al, J. Chem. Soc., Chem. Commun., 1989, 1823 (synth)

Br_2NNb IC-001844

Niobium(*V*) bromide nitride ($NbBr_2N$), 10Cl

[62804-20-0]

$NbBr_2N$

M 266.7

Synth. by heating $NbBr_5$ + NH_4Br or $NbCl_5$ + NH_4Br to 210° then to 230° *in vacuo*. Dark-brick-red solid which slowly hydrol. in air.

Smirnova, S.M. et al, Russ. J. Inorg. Chem. (Engl. Transl.), 1977, 22, 402 (synth, ir, thermal anal)

Br_2NORu IC-001845

Dibromo(nitrosyl)ruthenium

$[Ru(NO)Br_2]_n$ ($n \geq 2$)

M 290.8

Struct. unknown; presumed polymeric. Prepd. by treating $[Ru(CO)_2Br_2]_n$ with NO at 230°. Dark brown solid.

Manchot, W. et al, Z. Anorg. Allg. Chem., 1933, 216, 99 (synth)

$Br_2N_2O_2W$ IC-001846

Dibromodinitrosyltungsten, 11Cl

[44518-81-2]

$[W(NO)_2Br_2]_n$

M 403.6

Polymeric zig-zag-chain struct. with bromine bridges. Synth. from BrNO and $W(CO)_6$ in CH_2Cl_2 or from BrNO and $W_2(CO)_8Br_2$. Good starting material for synth. of $W(NO)_2Br_2L_2$ where L = As, N or P donor. Dark green powder. Thermally stable, dec. > 100°. Stored under N_2. Sol. donor solvs. e.g. MeOH, MeCN, Me_2CO; insol. alkanes, C_6H_6, $CHCl_3$, CH_2Cl_2, CCl_4.

[30731-18-1]

Johnson, B.F.G., J. Chem. Soc. A, 1967, 475 (ir)
Inorg. Synth., 1970, 12, 264 (synth)
Dows, R., J. Chem. Soc., Dalton Trans., 1972, 508 (synth)

Br_2N_2OP IC-001847

Phosphorazidic dibromide, 10Cl

Azidodibromophosphine oxide.

Azidodibromooxophosphorus(V)

[69715-77-1]

$Br_2P(O)N_3$

M 248.8

Not purif. Synth. from $POBr_3$ + NaN_3/MeCN.

▷ Presumed explosive.

Dillon, K.B. et al, Inorg. Nucl. Chem. Lett., 1978, 14, 511 (synth, P-31 nmr)

Br_2N_3P IC-001848

Phosphorazidium dibromide, 10Cl

Azidodibromophosphine. Azidodibromophosphorus(III)

Phosphorus azide bromide ($P(N_3)Br_2$)

[69715-73-7]

$(N_3)PBr_2$

M 232.8

Not purif. Synth. from PBr_3 + NaN_3/MeCN. Dec. slowly in CH_2Cl_2.

▷ Presumed explosive.

Oxide: see *Phosphorazidic dibromide*, IC-001847.

Sulfide: see *Phosphorazidothioic dibromide*, IC-001849.

Dillon, K.B. et al, Inorg. Nucl. Chem. Lett., 1978, 14, 511 (synth, P-31 nmr)
Dillon, K.B. et al, J. Chem. Soc., Dalton Trans., 1980, 1056 (props)

Br_2N_3PS IC-001849

Phosphorazidothioic dibromide, 10Cl

Azidodibromophosphine sulfide.

Azidodibromothiooxophosphorus(V)

[69715-75-9]

$Br_2PS(N_3)$

M 264.8

Not purif. Synth. from $PSBr_3$ + NaN_3/MeCN.

▷ Presumed explosive.

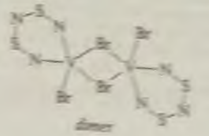
Dillon, K.B. et al, Inorg. Nucl. Chem. Lett., 1978, 14, 511 (synth, P-31 nmr)

$Br_2N_3S_2V$ IC-001850

[(Aminothio)sulfur diimidato(3−)-*N*,*N*′*]dibromovanadium(*V*), 11Cl

Cyclo-[(Disulfurtetraimide)dibromovanadium(V)]

[100286-36-0]



dimer

M 316.9

Dimeric.

Dimer:

$Br_4N_6S_4V_2$ M 633.8

Black solid. Mp 168° Subl$_{0.001}$ 130°.

Hanisch, J. et al, Z. Naturforsch., B, 1985, 40, 1457 (synth, cryst struct)
Roesky, H.W. et al, Z. Naturforsch., B, 1986, 41, 393 (synth, ir, V-51 nmr)

Br_2N_4Ti IC-001851

Diazidodibromotitanium(*IV*), 11Cl

Titanium azide bromide ($Ti(N_3)_2Br_2$)

[44800-45-5]

$TiBr_2(N_3)_2$

M 291.7

Synth. by adding IN_3 in CCl_4 to soln. of $TiBr_4$ in CCl_4. A similar reaction of $TiBr_4$ and Me_3SiN_3 in CH_2Cl_2 yields the product and a silyl polymer. Red-orange solid.

▷ V, explosive.

Wiberg, N. *et al, Chem. Ber.*, 1967, **100**, 748 (*synth from Me_3SiN_3*)
Dehnicke, K. *et al, Chem. Zig.*, 1982, **106**, 187 (*synth, ir*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3279 (*haz*)

IC-001852

Br_3NbO

Niobium(*IV*) bromide oxide ($NbBr_3O$), 11Cl

Niobium dibromide oxide

[103124-86-3]

$NbOBr_2$

M 268.7

Synth. by heating Nb foil, Nb_2O_5 and Br_2 in a sealed tube at 450/400°.

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1986, **534**, 209 (*synth*)

IC-001853

Br_3NbS

Niobium(*IV*) bromide sulfide ($NbBr_3S$), 11Cl

Niobium dibromide sulfide

[82546-45-0]

$NbBr_2S$

M 284.7

Synth. by disproportionation of Niobium(*V*) bromide sulfide ($NbBr_3S$). IC-001958 at 220°. Dark brown solid.

bin Baba, I., *Sains Malays.*, 1981, **10**, 69 (*synth*)

IC-001854

Br_3NbS_2

Niobium(*IV*) bromide sulfide ($NbBr_3(S_2)$), 9Cl

[12514-42-0]

$NbBr_3S_2$

M 316.8

Struct. comprises two square antiprisms bridged by 4Br, the S present as $S_2^{2\ominus}$ groupings on the remaining edges. Synth. by heating Nb + S + Br_2 in a sealed tube at 500/480°, or by heating Nb + S_2Br_2 at 500°. Solid. Thermal dec. yields NbS_3, S and $NbSBr_3$.

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1966, **347**, 225, 231 (*synth, thermal anal, cryst struct*)
Perrio, C. *et al, Bull. Soc. Chim. Fr.*, 1972, 3086 (*synth, ir, raman*)

IC-001855

Br_3NbSe_2

Niobium bromide selenide ($NbBr_3(Se_2)$), 10Cl

[67182-91-6]

$NbBr_3(Se_2)$

M 410.6

Chain struct. in which Nb forms pairs: $[Nb(\mu\text{-}Se_2)_2Nb(\mu\text{-}Br)_2]_n$ which account for the compound's diamagnetic semiconductor properties. Triclinic and monoclinic forms are known. Synth. by heating Nb, $NbBr_4$ and Se in a sealed ampoule at 480/475°. Violet-black solid.

Rijnsdorp, J. *et al, J. Solid State Chem.*, 1979, **30**, 365 (*synth, cryst struct, dec, pe*)

Br_3Nd

IC-001856

Neodymium bromide ($NdBr_3$)

Neodymium tribromide

[59323-04-1]

$NdBr_3$

M 304.0

Has $PbCl_2$ struct. Dark green cryst. Mp 725°.

Lueken, H. *et al, Rev. Chim. Minér.*, 1976, **13**, 113 (*magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6**, 9, 60 (*rev*)
Haschke, J.M., *Handbook on the Physics and Chemistry of Rare Earths*, 1979, **4**, 119 (*struct*)
Bratsch, S. *et al, Rare Earths Mod. Sci. Technol.*, 1982, **3**, 291 (*thermodyn*)

IC-001857

Br_3Ni

Nickel(*II*) bromide ($NiBr_2$)

Nickel dibromide

[13462-88-9]

$NiBr_2$

M 218.4

Anhydrous $NiBr_2$ has the CdI_2 struct. There is much confusion about authenticity of hydrates. Synth. from Ni or $Ni(CO)_4$ + Br_2 or by dehydration of hydrates. Commercially available as $NiBr_2.xH_2O$. Yellow cryst. Sol. H_2O; sl. sol. MeOH, EtOH, Me_2CO, Et_2O. Mp 963°. Paramagnetic.

Dihydrate: [13596-19-5].

Trihydrate: Yellow-green deliquescent needles. Sol. H_2O, EtOH, Et_2O. Loses $3H_2O$ at 300°.

Hexahydrate: [18721-96-5]. *Hexaaquanickel*(II) *dibromide*

$Br_2H_{12}NiO_6$ M 326.5

Probably bromide salt of Hexaaquanickel(*II*)(2+), IC-019897.

Nonahydrate: Probably bromide salt of Hexaaquanickel(*II*)(2+), IC-019897 with $3H_2O$ of crystallisation.

Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1433.
Remy, H., *Treatise on Inorg. Chem.*, Elsevier, 1956, **2**, 314.
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 351.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1687 (*synth*)

IC-001858

Br_4O

Bromine oxide (Br_4O)

Bromine monoxide. Dibromine oxide

[21308-80-5]

BrOBr

M 175.8

Spectra suggest bent molecule with C_{2v} symmetry. Formed by electric discharge on Br_2 + O_2 or from Br_2 + HgO. Yellow involatile solid at −63°, or dark brown liq., can be stored in CCl_4 at −30°. Sol. CCl_4, CCl_3F. Mp −17.5° dec.

▷ Dec. in CCl_4 to $COCl_2$ + Br_2 + Cl_2.

Schwarz, R. *et al, Chem. Ber.*, 1937, **70**, 1163 (*synth*)
Schwartz, R. *et al, J. Prakt. Chem.*, 1939, **152**, 157 (*synth*)
Schmeisser, M. *et al, Adv. Inorg. Chem. Radiochem.*, 1963, **5**, 70 (*props, bibl*)
Jolly, W.M., *Prep. Inorg. React.*, 1964, **1**, 246 (*rev*)
Radford, P.J.M. *et al, Bromine and its Compounds*, (Ed. Jolles), 1966, 147 (*rev*)
Campbell, C. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 888 (*synth, ir*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 317 (*synth*)
Ody, K. *et al, J. Chem. Soc., Perkin Trans. 2*, 1976, 521 (*synth*)
Pascal, J.L. *et al, CA*, 1977, **87**, 210447 (*struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 247.

Br_4OS

Thionyl bromide **IC-001859**

Sulfur(IV) *oxybromide. Sulfur*(IV) *dibromide oxide. Sulfinyl dibromide*

[507-16-4]

$Br_2S{=}O$

M 207.8

Interatomic distances: S—Br 227, S=O 145 pm. Synth. from $SOCl_2$ + HBr. Commercially available. Orange-yellow liq., slowly dec. on keeping. Hydrol. to HBr + SO_2. Sol. CS_2, CCl_4, $CHCl_3$, C_6H_6. d^{20} 2.685. Mp −52°. Bp 140°, Bp_{20} 48°.

Inorg. Synth., 1939, **1**, 113 (*synth*)
Mines, G.W. *et al, Proc. R. Soc. London, A*, 1972, **329**, 275 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 390 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 9, 1978, **B1**, 63 (*bibl*)

Br_4OSe

IC-001860

Seleninyl bromide, 11Cl, 10Cl, 9Cl

Selenium(IV) *oxybromide. Selenium dibromide oxide. Selenium*(IV) *bromide oxide ($SeBr_2O$)*

[7789-51-7]

$Br_2Se{=}O$

M 254.7

Probably pyramidal (C_s symmetry), interatomic distances: Se—O 163, Se—Br 236 pm. Synth. from SeO_2 + $SeBr_4$ or from $SeOCl_2$ + NaBr. Useful brominating agent. Colourless solid, dec. by moist air. Sol. org. solvs. d^{30} 3.38. Mp 41.6°. Bp_{740} 217° dec.

Lenher, V., *J. Am. Chem. Soc.*, 1922, **44**, 1668 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 10, 1949, **B**, 153; 1984, **B2**, 263 (*bibl*)
Milne, J., *Spectrochim. Acta, Part A*, 1982, **38**, 569 (*raman, synth*)

Br_4OTa

IC-001861

Tantalum(*IV*) bromide oxide ($TaBr_2O$), 11Cl

[98640-37-0]

$TaOBr_2$

M 356.7

Synth. from Ta + Ta_2O_5 + $TaBr_5$ in a temp. gradient (650-500°). Solid.

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1986, **534**, 209 (*synth, powder struct*)

Br_4OTh

IC-001862

Thorium bromide oxide ($ThBr_2O$)

Dibromooxothorium(IV). *Thorium dibromide oxide. Thorium*(IV) *oxybromide*

[13596-00-4]

$ThOBr_2$

M 407.8

Possesses the $UOCl_2$ struct. Obt. on heating hydrated $ThBr_4$ as well as from $ThBr_4$ + Sb_2O_3. White solid.

Chauvenet, E., *Ann. Chim. Phys.*, 1911, **8**, 425 (*synth*)

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 288 (*synth, ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1140 (*synth*)
Levet, J.C. *et al, J. Solid State Chem.*, 1979, **28**, 67 (*struct*)
Agarwal, B.K. *et al, Thermochim. Acta*, 1983, **63**, 363 (*synth*)
Corbett, J.D. *et al, J. Less-Common Met.*, 1986, **115**, 343 (*synth*)

Br_4OU

IC-001863

Uranium bromide oxide (UBr_2O)

Dibromooxouranium(IV). *Uranium oxybromide*(IV)

[19173-90-1]

$UOBr_2$

M 413.8

Possesses the $PaOCl_2$ struct. Synth. from UBr_4 + Sb_2O_3 at 400°, or from UO_2 + UBr_4 at 650°. Air-sensitive greenish-yellow cryst. Sol. H_2O. Paramagnetic, μ_{eff} = 3.27 μ_B (above 60K). Dec. >600° *in vacuo*.

Prigent, J., *Ann. Chim. (Paris)*, 1960, **13**, 65 (*synth*)
Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 288 (*synth, struct, ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1223 (*synth*)
Levet, J.C. *et al, J. Solid State Chem.*, 1979, **28**, 67 (*synth, ir, magnetism*)
Thibaut, E. *et al, J. Am. Chem. Soc.*, 1982, **104**, 5266 (*pe*)

Br_4OV

IC-001864

Vanadium(*IV*) bromide oxide (VBr_2O)

Dibromooxovanadium(IV)

[13520-89-3]

$[VOBr_2]_n$

M 226.7

Chains of *trans*-VO_2Br_4 octahedra share oxygen vertices. Synth. from $VOCl_3$ and BBr_3. $VOBr_2$ is formed in small amounts by thermal dec. of $[VBr_2(OH_2)_4]Br$. Solns. of V_2O_5 in HBr yield the dihydrate which may be dehydrated by heating to 160° in a stream of HBr. Astringent in antiperspirants.

Druce, P.M. *et al, J. Chem. Soc. A*, 1971, 3595 (*synth*)
Seifert, H.J. *et al, Z. Anorg. Allg. Chem.*, 1981, **479**, 32 (*synth, cryst struct*)
Bamberger, C.E. *et al, Inorg. Chim. Acta*, 1982, **57**, 161 (*synth*)
U.S. Pat., 4 490 354, (1984); *CA*, **102**, 100626b (*use*)

Br_4OW

IC-001865

Tungsten(*IV*) bromide oxide (WBr_2O)

Tungsten oxydibromide

[22445-32-5]

$WOBr_2$

M 359.6

Prepd. by heating stoichiometric amounts of W, WO_3 and Br_2. Grey-black shiny needles.

Tillack, J. *et al, Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 142 (*synth*)
Oppermann, H. *et al, Z. Anorg. Allg. Chem.*, 1972, **387**, 329 (*thermodyn*)
Inorg. Synth., 1973, **14**, 109 (*synth*)

Br_4OZr

IC-001866

Zirconium(*IV*) bromide oxide ($ZrBr_2O$)

Dibromooxozirconium(IV). *11Cl. Zirconyl bromide. Zirconium oxybromide*

[33712-61-7]

$ZrOBr_2$

M 267.0
Synth. by reaction of $ZrBr_4$ with Cl_2O in CCl_4 soln.
Catalyst for polyester condensation and in manuf. of polyethylene terephthalate. Also used in antiperspirants. White solid. Mp 350° dec. Dec. to ZrO_2 and $ZrBr_2$ at 350°. Forms adducts with O-donors by reaction in MeOH.

Dehnicke, K. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **331**, 121 (*synth*)
Japan. Pat., 71 27 551, (1971); *CA*, **76**, 26334 (*use, polym*)
Japan. Pat., 71 27 552, (1971); *CA*, **76**, 35172 (*use, polym*)
U.S. Pat., 3 927 188, (1975); *CA*, **82**, 155529 (*use*)
Srivastava, A.K. *et al*, *Croat. Chim. Acta*, 1981, **54**, 329 (*deriv, synth, ir*)
Srivastava, A.K. *et al*, *J. Indian Chem. Soc.*, 1981, **58**, 279 (*deriv, synth, ir*)
Agarwal, R.K. *et al*, *Thermochim. Acta*, 1983, **61**, 235 (*deriv, thermal anal*)

Br_2O_2U IC-001867

Uranium bromide oxide (UBr_2O_2)
Uranyl bromide. Dibromodioxouranium(VI)
[13520-80-4]

UO_2Br_2

M 429.8
Synth. from UBr_4 + O_2 at 170° or by electrochem. oxidn. Forms various complexes with Lewis bases. Thermally unstable bright red, hygroscopic solid. Sol. Me_2CO, Et_2O, EtOH, MeCN, H_2O. Bp 250° dec. Slowly loses Br_2 at r.t. Ir $\nu_{U=O}$ 948, 930, 905 cm^{-1}. ΔH_f −1136.1 kJ mol^{-1}.

Trihydrate:
$Br_2H_6O_5U$ M 483.8
Deliquescent dark yellow needles. Sol. H_2O, HBr aq. Loses Br_2 and turns red in air. Dec. at 115°, part of H_2O can be removed at 60° without dec., forms UO_3 >200°. Monohydrate and heptahydrate also reported.

Tris-THF complex: [110305-73-2].
$C_{12}H_{24}Br_2O_5U$ M 646.1
Light brown cryst. Sol. THF. 7-Coord. U.

Prigent, J., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1958, **247**, 1737.
Shchukarev, S.A. *et al*, *Zh. Neorg. Khim.*, 1958, **3**, 2651 (*synth*)
Shchukarev, S.A. *et al*, *Zh. Neorg. Khim.*, 1958, **3**, 2651 (*synth*)
Prigent, J., *Ann. Chim. (Paris)*, 1960, **5**, 65.
Prigent, J., *Ann. Chim. (Paris)*, 1960, **5**, 65.
Peterson, S., *J. Inorg. Nucl. Chem.*, 1961, **17**, 135 (*synth*)
Ellert, G.V. *et al*, *Zh. Neorg. Khim.*, 1965, **10**, 1572; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 858 (*synth, hydrate*)
Belyeav, Yu.I. *et al*, *Sov. Radiochem. (Engl. Transl.)*, 1967, **9**, 680.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1221 (*synth*)
Prins, G. *et al*, *J. Chem. Thermodyn.*, 1978, **10**, 1003.
Thibaut, E. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 5266 (*pe*)
Kumar, N. *et al*, *Inorg. Chim. Acta*, 1984, **95**, 211 (*synth, complexes*)
Rebizant, J. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 1298 (*THF complex, synth, cryst struct*)

Br_2O_3W IC-001868

Tungsten(*VI*) bromide oxide (WBr_2O_2)
Tungsten dibromide dioxide
[13520-75-7]

WO_2Br_2

M 375.6
Synth. from Br_2-O_2 mixt. and W, or by bromination of WO_3 with Br_2 or CBr_4. Red cryst. Disproportionates to WO_3 and $WOBr_4$ at 200-300°.

Pascal, P., *Nouveau Traité de Chimie Minérale*, Masson, Paris, 1959, **XIV**, 822.

Br_2O_3 IC-001869

Bromine oxide (Br_2O_3)
Dibromine trioxide
[53809-75-9]

OBrOBrO or $BrOBrO_2$

M 207.8
Formed by thermolysis of Br_2O_4 at 10^{-2} mmHg. Unstable, not fully characterised.

Mellor Compr. Treat. Inorg. Theor. Chem., 1922, **2**, 285; *Suppl II, Part 1*, 1956, 747
Pascal, J.L., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **279**, 43 (*synth, ir, raman*)
Pascal, J.L. *et al*, *CA*, 1977, **87**, 210447 (*struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 247.

Br_2O_4 IC-001870

Bromine oxide (Br_2O_4)
Dibromine tetraoxide. Bromine dioxide dimer
[53723-86-7]

$O_2Br—BrO_2$

M 223.8
Dimer of the BrO_2 radical. Synth. from Br_2 + O_3 in freon at −50°. Orange-yellow solid, dec. at 0°.

Schmeisser, M. *et al*, *Angew. Chem.*, 1959, **71**, 523 (*synth*)
Buxton, G.V. *et al*, *Proc. R. Soc. London, A*, 1968, **304**, 427 (*kinetics of dec*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 247.

Br_2O_6Pb IC-001871

Lead(*II*) bromate(*V*) ($Pb(BrO_3)_2$)
[34018-28-5]

$Pb(BrO_3)_2$

M 463.0
Colourless monoclinic cryst. + $1H_2O$. Sl. sol. cold H_2O (1.38 g per 100 cm^3). Dec. at 180°; (165° *in vacuo*); dehydrates at 95°.
▷ Toxic; may be explosive when impure, esp. during synth.

Gawande, A.M. *et al*, *Indian J. Chem., Sect. A*, 1979, **18**, 16 (*synth*)
Gawande, A.M. *et al*, *Therm. Anal., Proc. Int. Conf., 7th, 1982*, 1982, **1**, 693.
Lutz, H.D. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **529**, 46 (*ir*)

Br_2O_6Zn IC-001872

Zinc bromate ($Zn(BrO_3)_2$)
[14519-07-4]

$Zn(BrO_3)_2$

M 321.1
Cryst. V. sol. H_2O.
Hexahydrate: [13517-27-6]. *Hexaaquazinc(2+) bromate*
Synth. from $Ba(BrO_3)_2$ and $ZnSO_4$. Cryst. (H_2O). Mp *ca.* 100°. Cubic. struct. comprises discrete $[Zn(OH_2)_6]^{2\oplus}$ and $BrO_3^{\ominus}$ ions. Dehydration occurs at 200°.

Yu, S.H. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1936, **95**, 426 (*cryst struct, hexahydrate*)
Rolla, M., *Gazz. Chim. Ital.*, 1939, **69**, 779 (*synth, raman*)
Couture, L. *et al*, *Ann. Phys.*, 1948, **3**, 521 (*raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 893 (*rev, bibl*)
Rocchiccioli, C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **249**, 236 (*ir, hexahydrate*)

Ramaprabhu, S. *et al*, *Pramana*, 1984, **23**, 141 (*Br-79 nqr, hexahydrate*)
Sasidhar, Y.U. *et al*, *Cryst. Lattice Defects Amorphous Mater.*, 1986, **13**, 125 (*pmr, hexahydrate*)

Br_2O_8U IC-001873

Uranyl bromate

$UO_2(BrO_3)_2$

M 525.8
Obt. as monohydrate.
Monohydrate:
$Br_2H_2O_9U$ M 543.8
Hygroscopic fluorescent green-yellow powder. Ir $\nu_{U=O}$ 937, 954 cm^{-1} (ν_{sym} 878 cm^{-1}). Dec. at 203°.

Rammelsberg, C., *Pogg. Ann.*, 1842, **55**, 69 (*synth*)
Wergel, F. *et al*, *J. Less-Common Met.*, 1983, **91**, 359 (*synth, ir, dta*)

$Br_2O_{11}Sb_2$ IC-001874

Antimony bromide oxide ($Sb_2Br_2O_{11}$), 8Cl
[12323-33-0]

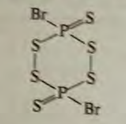
$Sb_2Br_2O_{11}$

M 1309.8
Synth. from $SbBr_3$ + Sb_2O_3. Monoclinic cryst.

Nurgaliev, B.Z. *et al*, *Zh. Neorg. Khim.*, 1981, **26**, 1043; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 564 (*synth, cryst struct*)

$Br_2P_2S_6$ IC-001875

Phosphorus bromide sulfide ($P_2Br_2S_6$)
3,6-Dibromo-1,2,4,5,3,6-tetrathiadiphosphorinane 3,6-disulfide. Diphosphorus dibromide hexasulfide

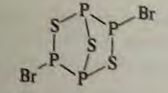


M 414.1
Interatomic distances: P—Br 207, P—S 210, S—S 203, P=S 198 pm. Synth. from P_4S_7 + Br_2 in CS_2. Tetragonal large opaque yellow needles. Mp 118° dec.

Andrews, J.M. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **25**, 829 (*synth, ir*)
Einstein, F.W.B. *et al*, *Inorg. Chem.*, 1965, **4**, 186 (*cryst struct*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 1168 (*rev*)

$Br_2P_4S_3$ IC-001876

Phosphorus bromide sulfide ($P_4Br_2S_3$)
3,6-Dibromo-2,5,7-trithia-1,3,4,6-tetraphosphabicyclo[2.2.1]heptane, 9Cl
[58878-07-2]



M 379.9
Synth. from corresp. diiodide + AgBr. Solid. Mp 55-58°.

Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **420**, 247 (*synth, P-31 nmr*)
Tattershall, B.W., *J. Chem. Soc., Dalton Trans.*, 1987, 1515 (*P-31 nmr*)

Br_2Pb IC-001877

Lead(*II*) bromide ($PbBr_2$), 9Cl
Lead dibromide
[10031-22-8]

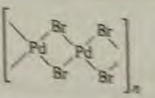
$PbBr_2$

M 367.0
$PbCl_2$ type struct. Synth. from PbO or $PbCO_3$ + HBr. Can also be formed directly from Pb + Br_2. Used as a photopolym. catalyst, a welding flux, in photoduplication processes, and in ir-transmitting glasses. White cryst. Sol. H_2O. Insol. EtOH. Mp 373°, Bp 916°.
▷ Toxic.
[30913-92-9]

Doell, W. *et al*, *Z. Anorg. Allg. Chem.*, 1939, **240**, 239 (*cryst struct*)
Hadni, A. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 1167 (*ir*)
Andersson, A. *et al*, *Acta Chem. Scand.*, 1970, **24**, 2670 (*cryst struct, hydrate*)
Willemsen, B., *J. Inorg. Nucl. Chem.*, 1971, **33**, 3963 (*raman*)
Dautov, G. *et al*, *Izv. Otd. Khim. Nauki, Bulg. Akad. Nauk*, 1974, **7**, 71; *CA*, **81**, 57684c (*synth*)
Ganz, G.J. *et al*, *J. Phys. Chem. Ref. Data*, 1977, **6**, 409 (*propr, molten*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **14**, 163.
Demidov, A.V. *et al*, *Zh. Strukt. Khim.*, 1983, **24**, 9; *CA*, **98**, 167378q (*struct, gaseous*)
Sharma, S. *et al*, *Z. Naturforsch., A*, 1987, **42**, 1313 (*Pb-207 nmr*)

Br_2Pd IC-001878

Palladium(*II*) bromide ($PdBr_2$), 8Cl
Palladium dibromide
[13444-94-5]



M 266.2
Polymeric struct. (α-$PdCl_2$ type) with square planar Pd. Synth. from Palladium, IC-021791 + Br_2. Commercially available. Red-black solid. Sol. HBr (aq.); insol. H_2O.

Wells, A.F., *Structural Inorg. Chem.*, 5th Ed., Oxford, 414 (*struct*)
Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1560.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1730 (*synth*)

Br_2Po IC-001879

Polonium(*II*) bromide ($PoBr_2$)
Polonium dibromide

$PoBr_2$

M 369.7
Formed from $PoBr_4$ by heating or by reduction with H_2S. Purple-brown solid. Disporportionates at its Mp. Mp 270-280° dec. $Subl._{30}$ 110°.

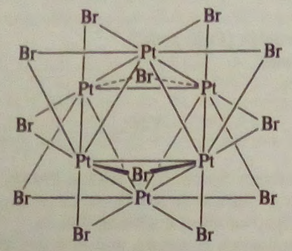
Bagnall, K.W. *et al*, *J. Chem. Soc.*, 1956, 3959 (*synth*)
Bagnall, K.W., *The Chemistry of Se, Te, Po*, Elsevier, 1966, 104 (*rev*)

Br_2Pt IC-001880

Platinum(*II*) bromide ($PtBr_2$), 9CI

Dodeca-μ-bromohexaplatinum(II). *Platinum dibromide*

[13455-12-4]



M 354.8

Struct. comprises Pt_6Br_{12} units. Synth. from H_2PtBr_4 or H_2PtBr_6 heated. Starting material for other $Pt^{(II)}$ Br compds. Commercially available. Brown solid. Sol. $Br^{\ominus}$ aq. Dec. at 230°.

Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1582.

Wells, A.F., *Structural Inorg. Chem.*, 5th Ed., Oxford, 1984, 414 (*struct*)

Br_2Rh IC-001881

Rhodium bromide ($RhBr_2$), 8CI

Rhodium dibromide

[19166-82-6]

$RhBr_2$

M 262.7

The gaseous molecule is said to have an angular struct. No recent studies; may not be genuine. Sol. H_2O.

Dwyer, F.P. *et al*, *J. Proc. R. Soc. N.S.W.*, 1941, **75**, 421 (*synth, props*)

Charkin, O.P. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1965, **6**, 550 (*struct*)

Br_2S IC-001882

Sulfur(*II*) bromide (SBr_2)

Sulfur dibromide. Dibromosulfane. Sulfurous bromide

[14312-20-0]

SBr_2

M 191.8

Formed by heating $[SBr_3]^{\oplus}[AsF_6]^{\ominus}$. Unstable compd., not fully characterised.

Gmelin Handbook Inorg. Chem., Syst. No. 9, 1978, **B2**, 293 (*bibl*)

Minkowitz, R. *et al*, *Z. Naturforsch., B*, 1986, **41**, 784 (*ms*)

Br_2SSi IC-001883

Dibromothioxosilane

Silicon dibromide sulfide

[13520-74-6]

$SSiBr_2$

M 219.9

Colourless plates. Sol. CS_2, C_6H_6; dec. in H_2O. Mp 93°. $Bp_{18.3}$ 150°.

Kirilenko, V.V. *et al*, *Fiz. Khim. Steckla*, 1975, **1**, 230 (*synth*)

Br_2SW IC-001884

Tungsten(*IV*) bromide sulfide (WBr_2S), 9CI

[54760-65-5]

$WSBr_2$

M 375.7

Struct. not detd. Synth. from Sb_2S_3 and WBr_5 at 140°. Brown solid.

Britnell, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2191 (*synth*)

Br_2S_2 IC-001885

Sulfur bromide (S_2Br_2), 11CI, 10CI, 9CI

Disulfur dibromide. Dibromodisulfane

[13172-31-1]

BrS—SBr

M 223.9

Interatomic distances: S—S 198, S—Br 224 pm; angle: BrSS 105°. Synth. by reaction of S + Br_2 or S_2Cl_2 + HBr. Red solid or dark red liq., dissociates on heating. Hydrol. to HBr + SO_2 + S. Sol. CCl_4, C_6H_6, CS_2. Mp −46°. With HBr gives sulfur chains S_xBr_2.

▷ Violent reaction with K, Na, Al and Sb, also with Fe at 650°. When moist, reacts violently with oxidants.

Hirota, E., *Bull. Chem. Soc. Jpn.*, 1958, **31**, 130 (*struct*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 386 (*synth*)

Gmelin Handbook Inorg. Chem., Syst. No. 9, 1978, **B2**, 293 (*bibl*)

Kniep, R. *et al*, *Z. Naturforsch., B*, 1983, **38**, 1 (*cryst struct*)

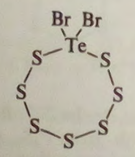
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1505 (*haz*)

Br_2S_7Te IC-001886

8,8-Dibromocycloheptathiatellurium

8,8-Dibromo-8,8-dihydroheptathiatellurocane, 10CI

[39943-94-7]



M 511.8

Formed from $TeBr_4$ + H_2S_n. Brown air-sensitive cryst.

Weiss, J. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 3653 (*synth, cryst struct*)

Br_2Se IC-001887

Selenium(*II*) bromide ($SeBr_2$)

Selenium dibromide. Dibromoselane

[22987-45-7]

$SeBr_2$

M 238.7

Not isol. but present in the vapour of Se_2Br_2 and $SeBr_4$. Interatomic distance: Br—Se 232 pm; angle: 100°.

Gmelin Handbook Inorg. Chem., Syst. No. 10, 1949, 149; 1984, **B2**, 234 (*complexes*)

Wynne, P.S. *et al*, *Inorg. Chem.*, 1972, **11**, 1192 (*ir, raman*)

De Leeuw, D.M. *et al*, *Chem. Phys.*, 1979, **38**, 21 (*pe*)

Br_2SeW IC-001888

Tungsten(*IV*) bromide selenide (WBr_2Se)

[54760-66-6]

$WSeBr_2$

M 422.6

Synth. by disproportionation of $WSeBr_3$ at 220°.

Britnell, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2191 (*synth*)

Br_2Se_2 IC-001889

Selenium bromide (Se_2Br_2), 11CI, 10CI, 9CI

Diselenium dibromide. Dibromodiselane. Selenous bromide

[7789-52-8]

BrSe—SeBr

M 317.7

Exists in 2 cryst. forms as solid. Ionises in solvs. such as MeCN. Synth. from Se + Br_2 in CS_2. Commercially available. Dark-red oily liq. Dec. slowly by H_2O to SeO_2 + Se + HBr. Readily disproportionates to Se + $SeBr_4$. Sol. disulfuric acid, CCl_4, CS_2. d^{15} 3.604. Bp 225-230° dec.

α-form

Interatomic distances: Se—Se 194.8, Br—Se 223.7 pm; angle: BrSeSe 109.2°. Mp 5°.

β-form

Interatomic distances: Se—Se 224.1, Br—Se 236.6 pm; angle: BrSeSe 103.9°. Brown-black solid. Mp 5°.

[12049-00-2]

Gmelin Handbook Inorg. Chem., Syst. No. 10, 1949, 147; 1984, **B2**, 222 (*rev, bibl*)

Stammreich, F.G.H. *et al*, *Spectrochim. Acta*, 1956, **8**, 46 (*ir, raman*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 418 (*synth*)

Kniep, R. *et al*, *Z. Naturforsch., B*, 1983, **38**, 1 (*cryst struct*)

Milne, J., *J. Chem. Soc., Chem. Commun.*, 1991, 1048 (*Se-77 nmr*)

Br_2Sm IC-001890

Samarium bromide ($SmBr_2$)

Samarium dibromide

[50801-97-3]

$SmBr_2$

M 310.1

Has $PbCl_2$ struct. as brown form. Black form ascribed $SrBr_2$ struct. Brown solid (also obt. as black solid, dark green powder). Dec. by H_2O. Mp 700° (669°, 508°). Bp 1880°.

Klemm, W. *et al*, *Z. Anorg. Allg. Chem.*, 1928, **176**, 181 (*synth*)

Döll, W. *et al*, *Z. Anorg. Allg. Chem.*, 1939, **24**, 239 (*synth*)

Spedding, F.H. *et al*, *Metall. Rev.*, 1960, **5**, 297 (*synth*)

Baeringhausen, H., *Rev. Chim. Minér.*, 1973, **10**, 77 (*cryst struct*)

Haschke, J.M., *Inorg. Chem.*, 1976, **15**, 298 (*struct, synth*)

Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6**, 64 (*rev*)

Wood, E.B. *et al*, *Rare Earths Mod. Sci. Technol.*, 1982, **3**, 153 (*uv-vis*)

Br_2Sn IC-001891

Tin(*II*) bromide ($SnBr_2$), 9CI

Stannous bromide. Tin dibromide

[10031-24-0]

$SnBr_2$

M 278.5

Synth. by dissolving Sn in conc. HBr. Bright yellow cryst., somewhat hygroscopic and light-sensitive. Hydrol. by H_2O. Sol. H_2O, EtOH, Et_2O, Me_2CO. Mp 215.5°. Bp 620°.

Kendall, J. *et al*, *J. Am. Chem. Soc.*, 1923, **45**, 963 (*synth*)

Wittig, G. *et al*, *Chem. Ber.*, 1939, **72**, 1387 (*synth*)

Knowles, D.J. *et al*, *J. Phys. Chem.*, 1970, **74**, 3642 (*ms*)

Andersson, J. *et al*, *Acta Chem. Scand., Ser. A*, 1975, **29**, 956 (*cryst struct*)

Donaldson, J.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 996 (*mössbauer*)

Deans, R.A. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1978, **8**, 345 (*synth*)

Gospodinov, G.G., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1984, **29**, 1407 (*synth*)

Br_2Sr IC-001892

Strontium bromide ($SrBr_2$), 8CI

[10476-81-0]

$SrBr_2$

M 247.4

Struct. type $SrBr_2$ characterised by 7- and 8-coord. Sr atoms and trigonally and tetrahedrally coord. Br atoms. May be considered a hybrid of $SrCl_2$ and SrI_2 struct. Synth. in high purity from Sr + $[NH_4]Br$ in liq. NH_3. Cryst. from aq. soln. yields the hexahydrate which is fully dehyd. at 180°. Hygroscopic white tetragonal cryst. V. sol. H_2O (100 g per 100 cm^3 at 20°; 223 g per 100 cm^3 at 100°); sol. EtOH. Mp 657°. ΔH_f° −718 kJ mol^{-1}; ΔG_f° −699 kJ mol^{-1}; S° 143 J K^{-1} mol^{-1}.

▷ WK8050000.

Monohydrate: [33429-50-4].

Br_2H_2OSr M 265.4

Formed during thermal dec. of hexahydrate.

Hexahydrate: [7789-53-9].

$Br_2H_{12}O_6Sr$ M 355.5

Colourless hexagonal cryst., dec. on heating with H_2O loss (−5 H_2O at 89°; −6H_2O at 180°). V. sol. H_2O (204 g per 100 cm^3 at 0°). ΔH_f° −2531 kJ mol^{-1}; ΔG_f° −2175 kJ mol^{-1}; S° 406 J K^{-1} mol^{-1}.

▷ WK8225000.

Swanson, H.E. *et al*, *Natl. Bur. Std. Circ. 539*, 1955, **4**, 60 (*cryst struct, hexahydrate*)

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **19**, 50 (*uses*)

Smeggil, J.G. *et al*, *Inorg. Chem.*, 1971, **10**, 1458 (*cryst struct*)

Lutz, H.D. *et al*, *Z. Naturforsch., B*, 1973, **28**, 8 (*thermal dec, hexahydrate*)

Hadenfeldt, C., *Z. Naturforsch., B*, 1975, **30**, 165 (*synth*)

Lutz, H.D. *et al*, *J. Mol. Struct.*, 1982, **96**, 61 (*ir, raman, monohydrate*)

Lutz, H.D., *Spectrochim. Acta, Part A*, 1982, **38**, 921 (*ir, raman, hexahydrate*)

Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 490 (*thermochem data*)

Br_2Ta IC-001893

Tantalum(*II*) bromide ($TaBr_2$), 11CI

Tantalum dibromide

[13569-48-7]

$TaBr_2$

M 340.7

Struct unknown; possibly exists as Ta_6Br_{12}. Synth. by H_2 reduction of $TaBr_5$ at 245-280°. Reduction with Ta only gives a mixture of $TaCl_3$ and $TaCl_2$. Pale blue solid.

Berdonosov, S.S. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, **7**, 1125 (*synth*)
Dittmer, G. *et al*, *Philips J. Res.*, 1985, **40**, 55; *CA*, **103**, 201767z (*transport props, thermodyn*)

IC-001894

Br_2Te

Tellurium(*II*) bromide ($TeBr_2$)
Tellurium dibromide
[7789-54-0]

$TeBr_2$

M 287.4
Synth. from Te + $TeBr_4$ in CF_2Br. Amorphous brown solid, disproportionates in H_2O, liq. SO_2, and on heating. Dec. in light. Sol. org. solvs.

Aynsley, E.E. et al, J. Chem. Soc., 1955, 2603 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 11, 1978, **B3**, 4 (*bibl*)

IC-001895

Br_2Ti

Titanium bromide ($TiBr_2$)
Titanium dibromide
[13783-04-5]

$TiBr_2$

M 207.6
CdI_2 struct. Synth. by disproportionation of $TiBr_3$ at ~350° or from $TiBr_4$ and Ti in a sealed tube at 800°. A v. reactive form results from thermol. of Me_2TiBr_2 in Et_2O. Black solid. Disproportionates to Ti and $TiBr_4$ above 400°. Mp > 500° dec. Paramagnetic. μ_{eff} = $1.29\mu_B$ (288K), $0.78\mu_B$ (90K).

Ehrlich, P. et al, Z. Anorg. Allg. Chem., 1961, **312**, 80 (*synth, cryst struct*)
Fowles, G.W.A. *et al*, *J. Chem. Soc. A*, 1968, 195 (*synth*)
Schlapfer, M. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **526**, 45 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3278.

IC-001896

Br_2Tm

Thulium bromide ($TmBr_2$)
Thulium dibromide
[64171-87-7]

$TmBr_2$

M 328.7
Has EuI_2 struct. Other polymorphs obt. at high temps. Dark green solid.

Korenistova, A.N., Zh. Neorg. Khim., 1977, **22**, 2130; 1979, **24**, 1139; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 1152; 1979, **24**, 633 (*sol-vol*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, Ok 75 (*rev*)
Hanchar, J.M., *Handbook on the Physics and Chemistry of Rare Earths*, 1979, **4**, 119 (*rev*)
Brauer, V., *CA*, 1985, **102**, 83736 (*struct*)

IC-001897

Br_2V

Vanadium bromide (VBr_2), 11Cl
Vanadium dibromide
[14896-41-6]

VBr_2

M 210.7
Hexagonal CdI_2 struct. Synth. from VBr_3 + H_2 at 450° in a flow system. Light brown-red solid, thermally stable to at least 900°. Paramagnetic. μ_{eff} = $2.86\mu_B$ (293K), $1.45\mu_B$ (90K). ΔH_f° −347 kJ mol^{-1}.

Klemm, W. *et al*, *Z. Anorg. Allg. Chem.*, 1942, **198**, 249 (*cryst struct*)
Shchukarev, S.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, **7**, 345 (*thermochem*)
McCarley, R.E. *et al*, *Inorg. Chem.*, 1964, **3**, 60 (*synth, thermodynamics*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1412 (*synth*)

IC-001898

Br_2Y_3

Yttrium bromide (Y_2Br_3)
Yttrium sesquibromide
[73728-20-8]

Y_2Br_3

M 426.5
Has Gd_2Cl_3 struct. in which metal octahedra share edges forming infinite chains. Synth. in low yield by heating YBr_3 and excess Y at 907°, cryst. at 747°. Fine needles.

Mattausch, H. *et al*, *Inorg. Chem.*, 1980, **19**, 2128 (*synth, cryst struct*)

IC-001899

Br_2Yb

Ytterbium bromide ($YbBr_2$)
Ytterbium dibromide
[25502-05-0]

$YbBr_2$

M 332.8
Exhibits several cryst. forms including SrI_2 and $CaCl_2$ structs. Can be synth. from Yb + 1,2-dibromoethane. Yellow or grey green solid. Sl. sol. THF; sol. H_2O. Mp 677° (673°). Bp 1800°. Dec. by H_2O. Exhibits red fluorescence in uv light.

Döll, W. *et al*, *Z. Anorg. Allg. Chem.*, 1939, **241**, 239 (*synth*)
Klemm, W. *et al*, *Z. Anorg. Allg. Chem.*, 1939, **241**, 239
Spedding, F.H. *et al*, *Metall. Rev.*, 1960, **5**, 297 (*synth*)
Beck, H.P. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **386**, 221 (*synth, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, Ok 75 (*rev*)
Hanchar, J.M., *Handbook on the Physics and Chemistry of Rare Earths*, 1979, **4**, 119.
Watson, P.L., *J. Chem. Soc., Chem. Commun.*, 1980, 652.

IC-001900

Br_2Zn

Zinc bromide ($ZnBr_2$)
[7699-45-8]

$ZnBr_2$

M 225.1
Tetragonal in solid state: Br in fcc array with Zn in ¼ of tetrahedral holes; isotypic with ZnI_2. Linear in gas phase. V. hygroscopic colourless cryst.; anhydrous (H_2O, > 37°), dihydrate (H_2O < 35°). Sol. H_2O (388 g per 100 cm^3). Mp 394°. Bp 650°.

▶ ZH1150000.

Sidgwick, E.J. *et al*, *J. Chem. Phys.*, 1935, **3**, 241 (*raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 885 (*rev, bib*)
Kiser, R.W. *et al*, *Adv. Chem. Ser.*, 1968, **72**, 153 (*rev*)
Beattie, I.R. *et al*, *J. Chem. Soc. A*, 1970, 2429 (*raman, gas*)
Mesaric, V. *et al*, *High Temp. High Pressures*, 1975, **7**, 439 (*phase trans*)
Susic, M.V. *et al*, *J. Chem. Phys.*, 1975, **62**, 744 (*struct, melt*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1025 (*synth*)
Wagner, C.D., *Faraday Discuss. Chem. Soc.*, 1976, **60**, 291 (*augers*)
Maciel, G.E. *et al*, *J. Phys. Chem.*, 1977, **81**, 263 (*Zn-67 soln nmr*)
Givan, A. *et al*, *J. Mol. Struct.*, 1978, **48**, 325 (*ir, raman, matrix*)

Bastow, T.J. *et al*, *Solid State Commun.*, 1980, **33**, 399 (*Br-nqr*)
Bristow, D.J. *et al*, *Chem. Phys.*, 1983, **75**, 263 (*pe*)
Goggin, P.L. *et al*, *Acta Chem. Scand., Ser. A*, 1984, **38**, 625 (*soln struct, raman, ir*)
Chieh, C. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1984, **166**, 189 (*cryst struct*)
Hargittai, M. *et al*, *Inorg. Chem.*, 1986, **25**, 3163 (*ed*)
Dent, P. *et al*, *J. Phys. Colloq.*, 1986, **C8**, 809 (*exafs*)
Yang, M.M. *et al*, *J. Solution Chem.*, 1988, **17**, 751 (*soln raman*)
Frahm, R. *et al*, *Physica B: (Amsterdam)*, 1989, **158**, 562 (*aq soln struct*)

IC-001901

Br_2Zr

Zirconium bromide ($ZrBr_2$), 11Cl
Zirconium dibromide
[24621-17-8]

$ZrBr_2$

M 251.0
Isostructural with $ZrCl_2$. Synth. by disproportionation of $ZrBr_3$ between 320° and 500°. Used as an absorber in artificial kidneys, (see also Zirconium bromide ($ZrBr_3$), IC-002003 and Zirconium bromide ($ZrBr_4$), IC-002090) and as anode in H_2/O_2 fuel cells. Blue-black solid which disproportionates to Zr + $ZrBr_4$ above 400°. ΔH_f −410kJ mol^{-1}.

Schäfer, H.L. *et al*, *Z. Elektrochem.*, 1962, **66**, 367 (*synth*)
Cotton, F.A. *et al*, *Halides of the Second and Third Row Transition Metals*, Wiley, New York, 1968 (*rev*)
Eysel, H.H. *et al*, *Journ. Int. Etude Piles Combust., C.R., 3rd.*, 1969, 82; *CA*, **76**, 134945q (*use*)
Marsh, G.S. *et al*, *Vestn. Mosk. Univ., Ser. 2: Khim.*, 1977, 1852; *CA*, **87**, 61808n (*synth, cryst struct*)
Br. Pat., 107 494, (1964); *CA*, **101**, 28336s (*use*)

IC-001902

$Br_3^{\ominus}$

Tribromide(1 −)
[14522-80-6]

$[Br—Br—Br]^{\ominus}$

M 239.7 (ion)
Linear, may or may not be symmetrical depending on counter cation. Used on polymer support as brominating agent. Forms red salts. Dissociates in H_2O. Linear symmetrical in $Me_3NH^{\oplus}$ salt. Br—Br 253 pm.
Cs salt: Synth. from conc. aq. CsBr and Br_2. Unsymmetrical anion, isostructural with CsI_3.
Tetrabromiphosphonium salt:
Br_9P M 590.3
Synth. from Cs_3, PBr_3 and Br_2. V. hygroscopic flat red needles. Loses bromine readily unless kept in soln. or sealed glass tube. Unsymmetrical anion: Br—Br 290, 230, angle BrBrBr 177.3°.
Me_4N salt: [15625-56-6].
Synth. from Me_4NBr and Br_2 in HOAc. Red-orange cryst. Mp 118-118.5°. Symmetrical anion: Br—Br 253 pm.
Et_4N salt: [6726-55-3].
Tetrabutylammonium salt: [38932-80-8].
Synth. from Bu_4NBr and Br_2. Light orange cryst. Mp 71-73°.
Benzyltrimethylammonium salt: [111865-47-5].
Brominating agent for org. compds.

Aldrich Chem. Co. Inc., Aldrich Catalog Handbook of Fine Chemicals, 1997, 167.
Brown, W.B. *et al*, *J. Chem. Phys.*, 1961, **35**, 908 (*ir, raman*)
Bowmaker, G.L. *et al*, *Acta Crystallogr.*, 1967, **23**, 334, 467 (*cryst struct PBr_4 salt*)
Evans, I.C. *et al*, *Inorg. Chem.*, 1967, **6**, 1483 (*raman*)
Gabes, W. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1971, **90**, 157 (*ir, raman, struct, asym anion*)
Hecquet, B. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1972, **274**, 1353 (*form const*)
Rallo, F. *et al*, *J. Electrochem. Soc.*, 1972, **119**, 1471 (*synth*)
Gabes, W. *et al*, *J. Mol. Struct.*, 1972, **14**, 267 (*ir, raman, struct*)
Kajigaeshi, S. *et al*, *Chem. Express*, 1988, **3**, 347 (*use*)
Gerischer, H. *et al*, *J. Electrochem. Soc.*, 1988, **135**, 2782 (*use*)
Bellucci, G. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 199 (*ir, form const*)
Tee, O.S. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 2233 (*bromination reactions*)
Behl, W.K., *Proc. Electrochem. Soc.*, 1989, **89** (*electrolytic synth*)

IC-001903

$Br_3^{\ominus}$

Tribromine(1 +)
[33105-86-1]

$[Br—Br—Br]^{\oplus}$

M 239.7 (ion)
Bent cation. Used as a brominating agent. Red cation. Dissociates in H_2O.
Hexafluoroarsenate: [12429-01-5].
$AsBr_3F_6$ M 428.6
Synth. from O_2AsF_3 and Br_2 or from Br_2, BrF_3 and AsF_3. Chocolate brown solid at r.t., carmine red at −195°. Subl. 30-50°. Dec. under N_2 at 70°.
Fluorosulfate: [58722-89-7].
Br_3FO_3S M 338.7
Synth. from Br_2 and $BrOSO_2F$ at low temp. Ir ν_{as} 288 cm^{-1}.
Tetrakis(fluorosulfato-O)aurate(1 −): [72030-47-0].
$AuBr_3F_4O_{12}S_4$ M 852.9
Synth. from Au and $BrSO_3F$. Dark brown hygroscopic polycryst. Dec. at 105°.
Bis(tetrafluorosulfato-O)platinate(2 −) (2:1): [90846-22-3].
$Br_6F_8O_{16}PtS_4$ M 1268.8
Synth. from Pt, excess $BrSO_3F$ and Br_2. Hygroscopic dark brown solid. Dec. on standing in air, dec. under N_2 at 90°.

Glemser, O. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 537 (*synth, ms, ir*)
Gillespie, R.J. *et al*, *Q. Rev., Chem. Soc.*, 1971, **25**, 553 (*rev*)
Gillespie, R.J. *et al*, *Inorg. Chem.*, 1972, **11**, 586 (*synth, raman*)
Wilson, W.W. *et al*, *J. Fluorine Chem.*, 1976, **7**, 245 (*ir, fluorosulfate*)
Brooks, W.V.F. *et al*, *Can. J. Chem.*, 1979, **57**, 3239 (*use*)
Lee, K.C. *et al*, *Inorg. Chem.*, 1980, **19**, 119; 1984, **23**, 2236 (*synth, arsenate salt, ir, raman*)
Chen, L.H. *et al*, *J. Raman Spectrosc.*, 1983, **14**, 232 (*raman*)

IC-001904

$Br_3CdI^{\ominus}$

Tribromoiodocadmate(1 −)
[21439-36-1]

$(CdBr_3)^{\ominus}$

M 352.1 (ion)
K salt: [14552-11-9]. *Cadmium potassium bromide iodide ($CdKBr_3I$)*
Br_3CdIK M 391.2
Phase in the KBr-$CdBr_2$ system. Cryst. Mp 360°.
Cs salt: [18585-55-8]. *Cadmium caesium bromide iodide ($CdCsBr_3I$)*
Br_3CdICs M 485.0
Phase in the CsBr—$CdBr_2$ system. Cryst. Mp 427°.

D'yakov, I.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1959, **4**, 422; 1964, **9**, 766 (*synth, K, Cs salts*)
Davies, J.E.D. *et al*, *J. Chem. Soc. A*, 1968, 2854 (*raman*)
Mueller, C.R. *et al*, *Acta Chem. Scand., Ser. A*, 1977, **31**, 649 (*cryst struct, Cs salt*)

Iyer, M.N. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 127 (*cryst struct, Rb salt*)
Asahi, T. *et al, Acta Crystallogr., Sect. C*, 1990, **46**, 2352 (*cryst struct*)

IC-001905

Br_3Ce
Cerium(*III*) bromide ($CeBr_3$)
Cerium tribromide
[7790-86-5]

$CeBr_3$

M 379.8
Has UCl_3 struct. White solid. Sol. H_2O, THF. Mp 722° (732°). Bp 1705°.
▷ FK5075000.
Heptahydrate: [7789-56-2].
$Br_3CeH_{14}O_7$ M 505.9
Colourless cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Prob. isostructural with corresp. chloride.

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*struct*)
Kost, M.E., *Zh. Neorg. Khim.*, 1957, **2**, 2689 (*synth*)
Mayer, I. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*heptahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Clever, R.B. *et al, J. Appl. Phys.*, 1969, **40**, 1151 (*magnetism*)
Sata, S., *J. Phys. Soc. Jpn.*, 1976, **41**, 913 (*pe*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6**, 59 (*rev*)
Skjeltorp, A.T., *J. Appl. Phys.*, 1978, **49**, 1567 (*magnetism*)
Uwamino, Y. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al, J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

IC-001906

Br_3Cf
Californium(*III*) bromide ($CfBr_3$)
Californium tribromide
[20758-68-3]

$CfBr_3$

M 491.7
Dimorphic. Synth. from Cf_2O_3/HBr at 675°. Green solid (dark amber at Mp.). Subl. 785°. Appears to dissociate reversibly to $CfBr_2$ + Br_2 at 675°.
Low temp.-form
Approximates to BiI_3 struct.
High temp.-form
Approximates to high-$CrCl_3$ struct. Stable >500°. Under pressure, transforms to $PuBr_3$ type struct.

[24297-29-8]

Fried, S. *et al, Inorg. Nucl. Chem. Lett.*, 1968, **4**, 495 (*synth*)
Peterson, J.R. *et al, Inorg. Nucl. Chem. Lett.*, 1972, **8**, 423 (*synth*)
Burns, J.H. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 743, 2497 (*synth, cryst struct*)
Young, J.P. *et al, Inorg. Chem.*, 1980, **19**, 2209 (*cryst struct, uv-vis*)
Peterson, J.R. *et al, Inorg. Chem.*, 1985, **24**, 2467 (*uv-vis, cryst struct*)

IC-001907

$Br_3ClFe^{\ominus}$
Tribromochloroferrate(*III*)(1−), 11Cl
[31189-14-4]

$[FeBr_3Cl]^{\ominus}$ (C_{3v})

M 323.1 (ion)
Pesticide.
Ph_4P salt: [10878-66-8].
Potom. catalyst.

Et_4N salt: [27981-99-3].
Clausen, C.A. *et al, Inorg. Chem.*, 1970, **9**, 220 (*ir, synth, mössbauer*)
Bhavsar, G.P. *et al, J. Mol. Struct.*, 1973, **16**, 343 (*ir*)

IC-001908

$Br_3ClP^{\oplus}$
Tribromochlorophosphonium
Tribromochlorophosphorus(1+), 9Cl

$[PBr_3Cl]^{\oplus}$

M 306.1 (ion)
Formed in PCl_3—Br_2 or PBr_3—Cl_2 mixtures in oleum or $HSFO_3$. Unstable to solvolysis. Existence of tetrahaloborates claimed.
Acetate:
$C_2H_3Br_3ClO_3P$ M 365.1
Liq. of poor stability.

[50807-53-9, 50807-54-0]

Finch, A. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1863 (*raman*)
Grimmer, A.R., *Z. Anorg. Allg. Chem.*, 1973, **400**, 105 (*P-31 nmr*)
Malhotra, K.C. *et al, Aust. J. Chem.*, 1975, **28**, 991 (*synth*)
Dillon, K.B. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1391 (*synth, P-31 nmr*)

IC-001909

Br_3ClSi
Tribromochlorosilane
Silicon bromide chloride ($SiBr_3Cl$). Silicon tribromide chloride
[13465-76-4]

$SiBr_3Cl$ (C_{3v})

M 303.2
Colourless liq. d_4^{25} 2.497. Mp −20.8°. Bp 126-128°. Dec. in H_2O.

Goubeau, J. *et al, Z. Anorg. Allg. Chem.*, 1969, **366**, 113 (*ir*)
Hoefler, F., *Z. Naturforsch., A*, 1971, **26**, 547 (*ir*)
Niemann, U. *et al, Z. Naturforsch., B*, 1975, **30**, 202 (*nmr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 680 (*synth*)
Sladkov, I.B. *et al, Zh. Fiz. Khim.*, 1982, **56**, 1032.

IC-001910

Br_3ClSn
Tribromochlorostannane
Tin bromide chloride ($SnBr_3Cl$). Tin tribromide chloride
[14779-73-8]

$SnBr_3Cl$ (C_{3v})

M 393.8
Synth. by mixing $SnCl_4$ and $SnBr_4$ in 1:3 ratio. Liq. d^{13} 3.12. Mp 1°. Labile in soln.

Cerf, C. *et al, Bull. Soc. Chim. Fr.*, 1964, 389, 2818 (*ir*)
Shult, D.E., *Diss. Abstr. Int., B*, 1977, **38**, 187.
Colton, R. *et al, Inorg. Chim. Acta*, 1982, **61**, 1 (*Sn-119 nmr*)

IC-001911

$Br_3Cl_2Cu^{3\ominus}$
Tribromodichlorocuprate(*II*)(3−)

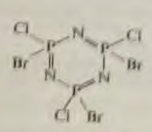
$[CuCl_2Br_3]^{3\ominus}$

M 374.1 (ion)
Trigonal bipyramidal. Bromine atoms disordered between axial and equatorial sites.
Hexamminechromium(3+) salt: [24858-76-2].
$Br_3Cl_2CrCuH_{18}N_6$ M 528.3
Dark red cryst.
Hexaamminecobalt(3+) salt: [38530-71-1].
$Br_3Cl_2CoCuH_{18}N_6$ M 535.2

Goldfield, S.A. *et al, Inorg. Chem.*, 1971, **10**, 2604 (*synth, cryst struct*)
Jeter, D.Y. *et al, J. Coord. Chem.*, 1972, **2**, 39 (*magnetism*)

IC-001912

$Br_3Cl_3N_3P_3$
2,4,6-Tribromo-2,4,6-trichloro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 8Cl
Tribromatrichlorocyclotriphosphonitrile. sym-Tribromotrichlorocyclotriphosphazene. 2,4,6-Tribromo-2,4,6-trichloro-2λ⁵,4λ⁵,6λ⁵-cyclatriphosphaza-1,3,5-triene. 2,4,6-Tribromo-2,4,6-trichloro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine
[16032-52-3]



M 481.0
Geometry unknown. Synth. from a mixture of $P_3N_3Cl_6$ and $P_3N_3Br_6$ heated to 250°. Solid. Mp 142°.

[6213-42-9, 19324-84-6]

Rotzsche, H. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 687 (*synth, gc*)
Steger, E. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 688 (*ir*)
Coxon, G.E. *et al, J. Chem. Soc. A*, 1969, 358 (*ms*)

IC-001913

$Br_3Cl_3Rh^{3\ominus}$
Tribromotrichlororhodate(*III*)(3−), 9Cl

$[RhBr_3Cl_3]^{3\ominus}$

M 448.9 (ion)
Octahedral: *fac*-isomer possible but not determined.
2,2',2''-Triammoniotriethylamine salt: [56604-55-8].
Light green solid, stable up to and above 300°.

Zipp, S.G. *et al, Inorg. Chim. Acta*, 1975, **14**, 83 (*synth, ir, uv*)

IC-001914

Br_3Cm
Curium(*III*) bromide ($CmBr_3$)
Curium tribromide
[14890-42-7]

$CmBr_3$

M 483.7
Possesses the $PuBr_3$ struct. Synth. from Cm_2O_3 + HBr. Pale yellow-green solid. Mp ~625°.

[24297-27-6]

Asprey, L.B. *et al, Inorg. Chem.*, 1965, **4**, 985 (*synth, cryst struct*)
Burns, J.H. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 743 (*synth, cryst struct*)

IC-001915

$Br_3Cr^{\ominus}$
Tribromochromate(*II*)(1−), 11Cl, 10Cl, 9Cl
[21910-39-4]

$[CrBr_3]_n^{n\ominus}$ chains

M 291.7 (ion)
Struct. analogous to Trichlorochromate(*II*)(1−), IC-016810. Salts obt. from melt or HOAc.
Antiferromagnetic.
K salt:
Br_3CrK M 330.8
Rb salt: [67303-59-9]. *Rubidium tribromochromate(II)* (*$RbCrBr_3$*)
Br_3CrRb M 377.1
Cs salt: [29794-91-0]. *Caesium tribromochromate(II)* (*$RbCrBr_3$*). *Caesium chromium bromide ($CsCrBr_3$)*
Br_3CrCs M 424.8
Brown, oxidises slowly in air.
Me_4N salt: [29794-92-1].
Yellow needles (HOAc). Antiferromagnetic.

Hanh, H.D. *et al, Z. Anorg. Allg. Chem.*, 1970, **373**, 93 (*synth, props*)
Li, T.-I. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 1539 (*cryst struct, uv, synth*)
Bellitto, C. *et al, Inorg. Chem.*, 1983, **14**, 1939 (*synth, magnetism, uv*)

IC-001916

Br_3Cr
Chromium(*III*) bromide ($CrBr_3$)
Chromium tribromide. Chromic bromide
[10031-25-1]

$CrBr_3$

M 291.7
BiI_3-type layer struct. Interatomic distance Cr—Br 257 pm. Can be synth. electrochemically using Cr anode and liq. Br_2. Dark green cryst. Easily oxidised in air; easily reduced by H_2. Insol. cold H_2O; sol. C_5H_5N. Mp 812° (1130° est.). μ_{eff} = 3.94μ_B (θ −51, 298K). Ferromagnetic. Begins to dissoc. at 700°.
Chromium(III) bromide hexahydrate [13478-06-3]
$Br_3CrH_{12}O_6$ M 399.7
Violet form: Hexaaquachromium(3+) tribromide
Blue-grey-violet cryst. V. sol. H_2O; insol. EtOH.
Green form: [82676-67-3]. *Tetraaquadibromochromium(1+) bromide dihydrate*
Synth. from CrO_3 and excess 50% HBr. Green deliquescent cryst.; stable in solid state. Sol. H_2O, EtOH; insol. Et_2O. On warming in soln., converts to violet form.

Gmelin Handbook Inorg. Chem., Syst. No. 52, 1962, **B**, 202 (*rev, bibl*)
Ferguson, J.E., *Halogen Chem.*, Academic Press, London, 1967, 3, 234 (*rev, bibl*)
Rupcheva, V.A. *et al, Zh. Neorg. Khim.*, 1970, **15**, 329; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 170 (*thermal dec*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1487 (*synth*)
Inorg. Synth., 1979, **19**, 123 (*electrochem synth*)
Klinkova, L.A. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1980, **16**, 1777; *Inorg. Materials (Engl. Transl.)*, 1980, **16**, 1207 (*props*)

IC-001917

Br_3CsPb
Caesium lead bromide ($CsPbBr_3$)
Caesium tribromoplumbate(II)
[15243-48-8]

$CsPbBr_3$

M 579.8
Perovskite struct. Synth. from $PbBr_2$ and CsBr. Pale orange prisms or needles. Phase transitions occur at 88° and 130°.

Wells, H.L., *Z. Anorg. Allg. Chem.*, 1893, **3**, 195 (*synth*)
Moller, C.K., *Nature (London)*, 1958, **182**, 1436 (*cryst struct*)
Eastesi, A.J., *Chem. Ind. (London)*, 1966, 600 (*synth*)
Hirotsu, S. *et al, J. Phys. Soc. Jpn.*, 1974, **37**, 1393 (*phase*)
Sakata, M. *et al, J. Phys. Soc. Jpn.*, 1979, **47**, 232 (*cryst struct*)
Hirshfeld, K. *et al, Phys. Rev. B*, 1981, **24**, 5942 (*spectra*)
Sharma, S. *et al, Z. Naturforsch., A*, 1987, **42**, 1313 (*Pb-207 nmr*)

Br_3CsSn IC-001918

Caesium tin bromide ($CsSnBr_3$)

Caesium tribromostannate(II)

[25150-43-0]

$CsSnBr_3$

M 491.3

Perovskite struct. Synth. from CsBr + $SnBr_2$. Black solid. Electrical conductor. Undergoes phase transitions at −26°, 1° and 19°.

Barrett, J. *et al*, *J. Chem. Soc. A*, 1971, 3105 (*synth*)
Bird, S.R.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1950 (*mössbauer*)
Bird, S.R.A. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 934 (*ir, raman*)
Scaife, D.E. *et al*, *J. Solid State Chem.*, 1974, **9**, 308 (*synth, nqr*)
Donaldson, J.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1500 (*cryst struct*)
Parry, D.E. *et al*, *J. Solid State Chem.*, 1979, **28**, 401 (*electronic struct*)
Mori, M. *et al*, *J. Phys. C*, 1986, **19**, 2391 (*phases*)
Yamada, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 4265 (*mössbauer, nqr*)

$Br_3Cu^{\ominus}$ IC-001919

Tribromocuprate(*II*)(1−)

[31415-59-5]

$[CuBr_3]^{\ominus}$

M 303.2 (ion)

Anion may be variously associated into eg. infinite $CuBr_4$ chains or dimers depending on counter-cation.

Cs salt: [16594-89-1]. *Caesium tribromocuprate*(II)
Br_3CsCu M 436.1

Isopropylammonium salt: Cryst. (EtOH). Three phase known: r.t. phase (III) contains chains of $[Cu_2Br_6]^{2\ominus}$ dimers; phase (II) contains $[CuBr_3]^{\ominus}$ and highest temp. phase (I) contains monobridged $[CuBr_4]^{2\ominus}$ tetrahedra.

Ph_4P salt: [88005-81-6].

Ludwig, W. *et al*, *Helv. Chim. Acta*, 1971, **54**, 1143 (*synth, uv, theory*)
Bastow, T.J. *et al*, *J. Mol. Struct.*, 1980, **58**, 305 (*nqr*)
Bloomquist, D.R. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 2615 (*synth, cryst struct, pmr, magnetism*)
Folkesson, B. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1983, **32**, 245 (*esca*)

Br_3Dy IC-001920

Dysprosium(*III*) bromide ($DyBr_3$)

Dysprosium tribromide

[14456-48-5]

$DyBr_3$

M 402.2

White solid. Sol. H_2O. Mp 881° (879°). Bp 1480°.

Hexahydrate: [14890-43-8].
Hexaaquadibromodysprosium(1+) bromide
$Br_3DyH_{12}O_6$ M 510.3
White cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Formulated as $[DyBr_2(OH_2)_6]^{\oplus}Br^{\ominus}$.

Mayer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*struct*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1968, 1889 (*hexahydrate, synth, cryst struct*)
Basile, L.J. *et al*, *J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, C6 (*rev*)
Friedt, J.M. *et al*, *Inorg. Chem.*, 1983, **22**, 2910 (*synth, mössbauer*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

Br_3Er IC-001921

Erbium(*III*) bromide ($ErBr_3$)

Erbium tribromide

[13536-73-7]

$ErBr_3$

M 406.9

Violet rose solid. Sol. H_2O, THF. Mp 950°. ~ 1460°°.

Hexahydrate: [14890-44-9]. *Hexaaquadibromoerbium(1+) bromide*
$Br_3ErH_{12}O_6$ M 515.0
Pink cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Formulated as $[ErBr_2(OH_2)_6]^{\oplus}Br^{\ominus}$.

Mayer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*hexahydrate, synth, cryst struct*)
Basile, L.J. *et al*, *J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, C6 (*rev*)
Legendziewicz, L.Z., *Bull. Pol. Acad. Sci., Chem.*, 1985, **33**, 147 (*uv-vis*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

Br_3Es IC-001922

Einsteinium(*III*) bromide ($EsBr_3$)

Einsteinium tribromide

[72461-17-7]

$EsBr_3$

M 491.7

6-Coord. with the $AlCl_3$ struct. Synth. from Es_2O_3 + HBr. Straw-coloured solid.

[57137-36-7]

Fellows, R.L. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 737 (*synth*)
Young, J.P. *et al*, *J. Radioanal. Chem.*, 1978, **43**, 479 (*synth*)
Young, J.P. *et al*, *Inorg. Chem.*, 1981, **20**, 3979 (*synth, uv-vis*)

Br_3Eu IC-001923

Europium(*III*) bromide ($EuBr_3$)

Europium tribromide

[13759-88-1]

$EuBr_3$

M 391.6

Has $PuBr_3$ struct. Light grey solid. Sol. H_2O. Mp 702°. Tends to dec. to $EuBr_2$ on heating.

Hexahydrate: [16021-75-3].
$Br_3EuH_{12}O_6$ M 499.7
Colourless monoclinic cryst. Sol. H_2O. Loses H_2O on controlled heating with formn. of EuOBr and some reduction to $Eu^{2\oplus}$.

Spedding, P.H. *et al*, *J. Chem. Phys.*, 1940, **8**, 908 (*hexahydrate, synth, uv-vis*)
Mayer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Haschke, J.M. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 2153 (*synth, cryst struct, hydrate*)
Deline, T.A. *et al*, *J. Chem. Thermodyn.*, 1975, **7**, 671 (*struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, C6, 70 (*rev*)
Lyle, S.J. *et al*, *Thermochim. Acta*, 1983, **68**, 51 (*hexahydrate, tga*)
Zolin, F. *et al*, *Koord. Khim.*, 1985, **11**, 1209; *CA*, **73**, 26320 (*hexahydrate, ir*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

Br_3FNO_2PS IC-001924

(Tribromophosphoranylidene)sulfamoyl fluoride, 8CI

Tribromophosphazosulfonyl fluoride. P,P,P-*Tribromo*-N-*(fluorosulfonyl)phosphazene.* P,P,P-*Tribromo*-N-*(fluorosulfonyl)phosphine imide*

[25077-35-4]

$Br_3P{=}NSO_2F$

M 367.7

Synth. from FSO_2NSO + PBr_5. Colourless solid. Mp 57-58°. $Bp_{0.05}$ 106-107°.

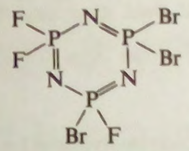
Roesky, H.W., *Z. Anorg. Allg. Chem.*, 1969, **367**, 151 (*synth, ir, F-19 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 9, *Sulfur-Nitrogen Compounds*, 1977, **1**, 122 (*rev, bibl*)

$Br_3F_3N_3P_3$ IC-001925

2,2,4-Tribromo-4,6,6-trifluoro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 8CI

gem-Tribromotrifluorocyclotriphosphonitrile. 2,2,4-Tribromo-4,6,6-trifluorocyclotriphosphazene. 2,2,4-Tribromo-4,6,6-trifluoro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2,4-Tribromo-4,6,6-trifluoro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine

[17022-77-4]



M 431.6

Synth. from $P_3N_3Br_6$ + AgF. Phys. props. not descr.

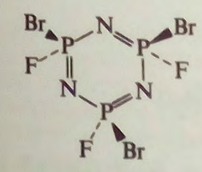
Steger, E. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1812 (*synth, ir, gc*)
Clare, P. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 467 (*ms, ir*)

$Br_3F_3N_3P_3$ IC-001926

2,4,6-Tribromo-2,4,6-trifluoro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 9CI

sym-*Tribromotrifluorocyclotriphosphonitrile. Tribromo-2,4,6-trifluorocyclotriphosphazene. 2,4,6-Tribromo-2,4,6-trifluoro-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,4,6-Tribromo-2,4,6-trifluoro-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine*

[67336-18-9]



cis-form

M 431.6

Synth. from $P_3N_3Br_6$ + AgF or from $P_3N_3F_3(NMe_2)_3$ + HBr. Bp 205°.

cis-form [38589-74-1]
(2α, 4α, 6α)-*form*
Irregular, slight chair conform. Orthorhombic. Interatomic distances: P—F 155.9, 151.9, P—Br 214.1, 217.7, P—N 158.9, 155.9 pm; angles: NPN 119.5, 118.8°, PNP 120.1, 118.8°, NPBr 110.8, 110.1, 110.5°, NPF 106.3, 107.4, 108.0°, FPBr 101.2, 98.5°. Cryst. Mp 76°.

trans-form [38589-75-2]
(2α, 4α, 6β)-*form*
Not obt. pure.

Clare, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 2374; 1975, 2071 (*synth, F-19 nmr, P-31 nmr*)
Clare, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2071 (*cryst struct*)
Clare, P. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 467, 477 (*ms, ir*)
Clare, P. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 883 (*ir, raman*)

$Br_3Fe^{\ominus}$

Tribromoferrate(*II*)(1−) IC-001927

$[FeBr_3]^{\ominus}$

M 295.5 (ion)

Salts do not contain discrete $[FeBr_3]^{\ominus}$ ions at least in solid state.

K salt: [54849-02-4]. *Potassium tribromoferrate*(II). *Iron*(II) *potassium bromide* ($FeKBr_3$)
Br_3FeK M 334.6
Paramagnetic at r.t. Isostructural with $KFeCl_3$.

Rb salt: [37473-39-5]. *Rubidium tribromoferrate*(II). *Iron*(II) *rubidium bromide* ($FeRbBr_3$)
Br_3FeRb M 381.0

Cs salt: [53899-57-3]. *Caesium tribromoferrate*(II). *Caesium iron*(II) *bromide* ($CsFeBr_3$)
Br_3CsFe M 428.4

Gurewitz, L. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2771 (*struct, magnetism*)
Briat, B. *et al*, *Raman Spectrosc., Proc. Int. Conf., 8th, 1982*, 8th, 1982, 421; *CA*, **99**, 148877f (*raman*)

Br_3Fe IC-001928

Iron(*III*) bromide ($FeBr_3$)

Ferric bromide

[10031-26-2]

$FeBr_3$

M 295.5

Near octahedral in solid state. Similar struct. to $FeCl_3$. Fe_2Br_6 dimer in gas phase. Synth. from $FeBr_2$ + Br_2 at elevated temp. or from Fe + Br_2. Forms adducts with a wide range of ligands. Lewis acid catalyst similar to Iron(*III*) chloride ($FeCl_3$), IC-016843. Bromination catalyst, e.g. in Friedel Crafts reactions. Red-brown cryst. Deliquescent. Dec. to iron(*II*) with ease at >120°. Sol. H_2O, EtOH, Et_2O, AcOH. Subl. with dec. on heating.

Hexahydrate: Ferric bromide hexahydrate
Obt. by recryst. of $FeBr_3$ from H_2O <49°. Dark green cryst. V. sol. H_2O, EtOH, Et_2O. Mp 27°.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 331 (*rev, bibl*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1934, **14**, 119 (*rev, bibl*)
Gregory, N.W. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3176; 1951, **73**, 472 (*synth, cryst struct*)
Sidgwick, *The Chemical Elements and their Compds.*, Oxford, 1950, **II**, 1332 (*rev, bibl*)
Druce, P.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 486 (*synth*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 3, 1963 (synth)
Gregory, N.W., *Inorg. Chem.*, 1988, **27**, 4294

IC-001829

Br_3Ga
Gallium(III) bromide ($GaBr_3$)
Gallium tribromide
[13450-88-9]

dimer

M 309.4
Dimeric
Dimer: Di-μ-bromotetrabromodigallium
Br_3Ga_2 M 618.8
Synth. from Ga + Br_2. White moisture-sensitive cryst. d^{25} 3.11. Mp 122.5°
Greenwood, N.N. *et al.*, *J. Inorg. Nucl. Chem.*, 1957, **3**, 332; 1958, **6**, 34 (prep)
Inorg. Synth., 1960, **6**, 31 (synth)
Greenwood, N.N. *et al.*, *Progr. Coord. Chem. Proc. Bienn. Conf. Chem.*, Glub, G.A., Ed. Interscience N.Y., 1963, **1**, 309 (rev)
Bell, A. *et al.*, *Trans. Faraday Soc.*, 1966, **62**, 721 (d, vapour)
Beattie, I.R. *et al.*, *J. Chem. Soc. A*, 1968, 813; 1969, 2654 (ir, raman)
Kimble, E. *et al.*, *J. Chem. Soc. A*, 1968, 460 (cr)
McGuire, G.E. *et al.*, *Inorg. Chem.*, 1973, **12**, 2450 (pe)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, Ferdinand Enke Verlag, 1975-1981, **2**, 857 (synth)

IC-001830

Br_3Gd
Gadolinium(III) bromide ($GdBr_3$)
Gadolinium tribromide
[13818-75-2]

$GdBr_3$

M 700.9
Can be used as neutron absorber shutdown material in nuclear reactors. White solid. Sol. H_2O. Mp 785°. μ_{eff} = 8.0μ_B (Curie-Weiss to 5K).
Hexahydrate: [13450-83-4].
$Br_3GdH_{12}O_6$ M 925.0
Colourless rhombic plates. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Isostructural with corresp. chloride.
Mayer, I. *et al.*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (hexahydrate, synth, pe)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (rev)
Brown, D. *et al.*, *J. Chem. Soc. A*, 1968, 1889 (hexahydrate, synth, cryst struct)
Yarovoi, F. *et al.*, *J. Chem. Phys.*, 1969, **50**, 5027 (magnetism)
Weigel, F. *et al.*, *Z. Anorg. Allg. Chem.*, 1970, **377**, 228 (struct)
Busch, L.J. *et al.*, *J. Chem. Phys.*, 1971, **55**, 3729 (e)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C8**, 71 (rev)
Beck, H.P. *et al.*, *Z. Anorg. Allg. Chem.*, 1983, **502**, 175 (struct)
Lokshynbina, N.S. *et al.*, *Zh. Fiz. Khim.*, 1984, **58**, 2631 (ir)
Ger. Pat., 3 133 859, (1985); *C.A.* **103**, 44008 (ser)
Umemoto, Y. *et al.*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (pe)
Meyer, G. *et al.*, *J. Less-Common Met.*, 1987, **127**, 155 (synth)

Br_3GeH IC-001831
Tribromogermane, 9CI
Germanium bromide hydride
[14779-70-5]

$GeHBr_3$

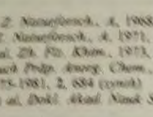
M 313.3
Formed together with $GeBr_4$ by reaction of HBr and Ge. Unstable liq. Mp −24°.
Brewer, F.M. *et al.*, *J. Phys. Chem.*, 1927, **31**, 1528 (synth)
Delwaulle, M.L. *et al.*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1950, **230**, 743 (synth)
Delwaulle, M.L. *et al.*, *J. Phys. Chem.*, 1952, **56**, 555 (raman)

Br_3HSi IC-001832
Tribromosilane
Silicobromoform. Silicon bromide hydride ($SiBr_3H$). Silicon tribromide hydride
[7789-57-3]

$SiHBr_3$ (C_{3v})

M 268.8
Interatomic distances: Si—H 149.4, Si—Br 217.0 pm; angle: BrSiBr 111.36°. Colourless liq. Sol. chlorinated hydrocarbons; dec. in H_2O, NH_3. d^{15} 2.7. Mp −73°. Bp 109°.
p- Flammable
Mitioff, M. *et al.*, *Z. Naturforsch., A*, 1948, **23**, 65
Hreenge, E. *et al.*, *Z. Naturforsch., A*, 1971, **26**, 768 (ir, pmr)
Sukovich, L.G. *et al.*, *Zh. Fiz. Khim.*, 1973, **47**, 1448
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 684 (synth)
Voronkov, M.G. *et al.*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **232**, 817 (ir)
Bunnell, J. *et al.*, *Spectrochim. Acta, Part A*, 1986, **42**, 543.

$Br_3H_2MoN_3O_3^{\ominus}$ IC-001833
Aquatribromodinitrosylmolybdate(1−), 11Cl
Dinitrosyltribromomolybdate(1−) monohydrate



M 413.6 (ion)
Approx. *mer*-octahedral anion.
Ph_4P salt: [85361-41-7].
Synth. from $MoBr_4$ + Br_3CNO + $[Ph_4P]Br$. Light green cryst. (CH_2Br_2). Sol. CH_2Br_2.
Schumacher, C. *et al.*, *Z. Anorg. Allg. Chem.*, 1982, **495**, 133 (cryst struct, synth, ir)

$Br_3H_2OZn^{\ominus}$ IC-001834
Aquatribromozincate(1−)
[18921-14-7]

$[ZnBr_3(OH_2)]^{\ominus}$

M 323.1 (ion)
X salt, monohydrate: [31371-00-3]. *Potassium zinc tribromide dihydrate*
Cryst. Mp 75°. Dimorphic: α-form, obtained from KBr and $ZnBr_2$ (1.75:1) in H_2O; β-form, obtained from KBr and $ZnBr_2$ (1:1) in H_2O.
[15279-57-9]

Epheritis, F., *Z. Anorg. Allg. Chem.*, 1969, **369**, 40 (synth, K salt)
Pellizer, G. *et al.*, *Acta Crystallogr., Sect. B*, 1969, **28**, 1359 (cryst struct, K salt, refine)
Ivlinskova, V. *et al.*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 555 (synth, conc)
Holmes, R. *et al.*, *Acta Crystallogr., Sect. B*, 1970, **26**, 1815 (synth, cryst struct, K salt, β-form)
Bobler, B. *et al.*, *Z. Anorg. Allg. Chem.*, 1974, **406**, 62 (cryst struct, Jr, K salt, refine)
Maciel, G.E. *et al.*, *J. Phys. Chem.*, 1977, **81**, 283 (ZFS, esr in SO_2)

Br_3H_2NZr IC-001835
Aminetribromodizirconium(III), 11Cl
Zirconium(III) bromide amine
[97459-08-0]

$(H_2N)Zr_2Br_3$

M 347.9
Synth. by heating $ZrBr_3.6NH_3$ to 100°. Dark grey solid. Paramagnetic. μ_{eff} = 0.85μ_B.
Boyle, E. *et al.*, *Inorg. Chim. Acta*, 1985, **100**, 281 (synth, magnetism, ir)

$Br_3H_2MnO_3^{\ominus}$ IC-001836
Diaquatribromomanganate(II)(1−)

$[MnBr_3(OH_2)_2]^{\ominus}$

M 330.6 (ion)
Synth. from 1:1 mixt. of aq. $MnBr_2$ and either CsBr or Me_3NHBr.
Cs salt: [59700-00-7]. *Caesium tribromomanganate(III) dihydrate*
$Br_3CsH_4MnO_2$ M 463.5
Struct. contains corner sharing chains of *cis*-$MnBr_4(H_2O)_2$ as in $CsNiCl_3.2H_2O$.
[50115-80-1]
Day, P. *et al.*, *J. Chem. Soc., Faraday Trans. 2*, 1973, **69**, 363 (synth, str-rel, struct)
McPherson, G.L. *et al.*, *J. Chem. Phys.*, 1974, **60**, 134 (synth)
Swiatt, C.H.W. *et al.*, *Physica (Amsterdam)*, 1974, **78**, 21 (magnetism)
Machani, S. *et al.*, *Physica (Amsterdam)*, 1974, **78**, 305 (synth, struct)
Yamamoto, I. *et al.*, *J. Phys. Soc. Jpn.*, 1977, **43**, 181 (magnetism)
Kopinga, K., *Phys. Rev. B*, 1977, **16**, 427 (magnetism)
Gmelin Handbook Inorg. Chem., Syst. No. 55, 1978, **C5**, 300; 1983, **C10**, 47 (ver, bibl, str-rel)

$Br_3H_2NO_3Ru$ IC-001837
Diaquatribromo(nitrosyl)ruthenium

$Ru(NO)Br_3(OH_2)_2$

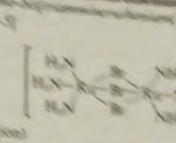
M 408.8
Struct. presumably *pseudo*-octahedral; isomeric form unknown. Prepd. by dissolving RuO_4 in an aq. HBr:HNO_3 mixt. Potentially v. valuable synth. reagent for complexes containing the $Ru(NO)Br_3$ moiety (cf. Diaquatrichloro(nitrosyl)ruthenium, IC-016865).
Joly, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **108**, 854 (synth)

$Br_3H_9N_3Ru$ IC-001838
Triamminetribromoruthenium(III), 9CI
Ruthenium(III) bromide triammine
[50216-73-8]

$Ru(NH_3)_3Br_3$

M 391.9
Only the *fac*-isomer known. Prepd. by aerial oxidation of $[Ru_2(NH_3)_6Br_6]Br_2$ or boiling *cis*-$[Ru(NH_3)_4Br_2]Br$ in conc. HBr. Sol. HBr. Thermal dec. → $2RuBr_3$ + 3NH$_3$ + $2NH_4Br$ + N_2 + H_2. D t_{max} 220, 310 (dta)
Glen, K. *et al.*, *Z. Anorg. Allg. Chem.*, 1939, **239**, 350 (synth)
Lever, F.M. *et al.*, *J. Chem. Soc. A*, 1969, 1477 (synth)
Tribalat, S. *et al.*, *J. Therm. Anal.*, 1969, **1**, 171 (thermal dec)
Bottomley, F. *et al.*, *Can. J. Chem.*, 1971, **49**, 2778 (synth)
Mercer, E.E. *et al.*, *J. Am. Chem. Soc.*, 1972, **94**, 6429 (synth)
Ohyoshi, A. *et al.*, *Chem. Lett.*, 1973, 1229 (thermal dec)
Durig, J.R. *et al.*, *J. Mol. Struct.*, 1973, **20**, 93 (ir, raman)

$Br_3H_{18}N_9Ru_2^{3\oplus}$ IC-001839
Hexaammine-tri-μ-bromodiruthenium(2+), 9CI
Tris-μ-bromo-bis[pentaamineruthenium(III)]
[58320-17-5]



M 544.0 (ion)
Originally incorrectly formulated as $[Ru_2(NH_3)_6Br_3(OH)_3]$ (μ-Br)Br. Sol. H_2O.
Tribromide
$Br_3H_{18}N_9Ru_2$ M 703.8
Prepd. by treating Hexaammineruthenium(2+), IC-020000 with conc. HBr. Blue-green cryst. μ_{eff} = 2.80 μ_B per dimeric unit.
Bottomley, F. *et al.*, *Can. J. Chem.*, 1971, **49**, 3778 (synth, reactions, magnetism)
Mercer, E.E. *et al.*, *J. Am. Chem. Soc.*, 1972, **94**, 6429 (preparation)
Durig, J.R. *et al.*, *J. Mol. Struct.*, 1973, **20**, 93 (ir, raman)

Br_3Hf IC-001840
Hafnium(III) bromide ($HfBr_3$), 11Cl
Hafnium tribromide
[13782-98-2]

$HfBr_3$

M 418.2
Struct. unknown. Synth. from $HfBr_4$ and Al at 430° and 80 atm. or from $HfBr_4$ and Hf at 460-530°and 40 atm. Blue-black solid which disproportionates above 330° to $HfBr_2$ and $HfBr_4$.
Schäfer, H.L. *et al.*, *Z. Anorg. Allg. Chem.*, 1967, **351**, 279 (synth)
Marek, G.S. *et al.*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1303 (synth)

$Br_3Hg_2O_3$ IC-001841
Mercury bromide oxide ($Hg_2Br_3O_3$)
[11129-20-5.5]

$Hg_2Br_3O_3$

M 1008.4

Mixed Hg(*I*)/Hg(*II*) compd. Struct. contains interlinked 12 membered rings of (Hg—Hg—O)$_4$ with $Br^\ominus$ in cavities. Synth. from Hg_2Br_2 and yellow HgO. Dark red-brown cryst.

Stalhandske, C., *Acta Chem. Scand., Ser. A*, 1987, **41**, 576 (*synth, cryst struct*)

IC-001942

Br_3Ho
Holmium(*III*) bromide ($HoBr_3$)
Holmium tribromide
[13825-76-8]

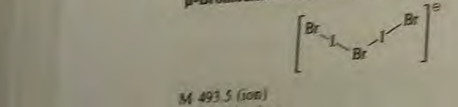
$HoBr_3$

M 404.6
Has YCl_3 struct. changing to $PuBr_3$ struct. under pressure. Yellow solid. Sol. H_2O, THF. Mp 914°. ~ 1470°°.
Hexahydrate: [15162-88-6]. *Hexaaquadibromoholmium(1+) bromide*
$Br_3H_{12}HoO_6$ M 512.7
Pale yellow cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Formulated as $[Ho(OH_2)_6Br_2]^\oplus Br$.

Mayer, I. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al, J. Chem. Soc., Dalton Trans.*, 1968, 1889 (*ankydr, hexahydrate, synth, cryst structs*)
Bastle, L.J. *et al, J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6** (*rev*)
Beck, H.P. *et al, Z. Anorg. Allg. Chem.*, 1983, **502**, 178 (*struct*)
Uwamino, Y. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al, J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

IC-001943

$Br_3I_2^\ominus$
μ-Bromodibromodiiodate(1−)



M 493.5 (ion)
V-shaped anion.
2,2'-Bipyridinium salt: [95547-80-1].
Synth. from 2,2'-bipyridinium bromide and BrI. Orange yellow solid.

Parlow, A. *et al, Z. Naturforsch., B*, 1985, **40**, 45 (*synth*)

IC-001944

$Br_3In^{2\ominus}$
Tribromoindate(*I*)(2−)
[38387-08-5]

$[InBr_3]^{2\ominus}$ (C_{3v})

M 354.5 (ion)
Synth. from $Me_2bipyBr_2$ and InBr in MeOH. Ir ν_{In-Br} 177, 149, 74, 46 cm^{-1}.
N,N'-Dimethyl-4,4'-bipyridinium(2+) salt: [35163-54-3].
Pale yellow solid (MeOH). Becomes blue on standing.

Contreras, J.G. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 1552
Contreras, J.G. *et al, Inorg. Chem.*, 1972, **11**, 2967 (*theory, raman*)
Contreras, J.G. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 922 (*synth, raman*)

IC-001945

Br_3In
Indium(*III*) bromide ($InBr_3$)
Indium tribromide
[13465-09-3]

$InBr_3$

M 354.5
In solid state has distorted NaCl struct. with $\frac{1}{3}$ metal ions missing; dimeric in melt and monomer-dimer eqm. in gas phase. Synth. from In and Br_2, purified by subl. Colourless solid becomes yellow below Mp. Mp 420°, 435°. Subl. 371°. Many complexes descr.

Walter, P.H.L. *et al, J. Inorg. Nucl. Chem.*, 1961, **19**, 223 (*synth, powder struct*)
Motawietz, W. *et al, Z. Anorg. Allg. Chem.*, 1962, **316**, 220 (*synth*)
Carty, A.J. *et al, J. Chem. Soc. A*, 1966, 1081 (*complexes*)
Greenwood, N.N. *et al, J. Chem. Soc. A*, 1969, 2655 (*ir, raman*)
Beattie, I.R. *et al, J. Chem. Soc. A*, 1969, 2654 (*ir, raman*)
Brown, D.H. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 3751 (*complexes*)
McGuire, G.E. *et al, Inorg. Chem.*, 1973, **12**, 2450 (*pe*)
Davies, J.E. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 805 (*raman*)
Nichols, G.D. *et al, Inorg. Nucl. Chem. Lett.*, 1979, **15**, 401 (*pe*)
Inorg. Synth., 1979, **19**, 257 (*synth*)

IC-001946

Br_3Ir
Iridium(*III*) bromide ($IrBr_3$), 8Cl
Iridium tribromide
[10049-24-8]

$IrBr_3$

M 431.9
insol.-form
Has $CrCl_3$ type struct. Mustard grey solid. Insol. alcohols, H_2O, acids.
sol.-form
Formed when $IrO_2.nH_2O$ is repeatedly evaporated to dryness with HBr. Sol. alcohols.

Angoletta, M. *et al, Gazz. Chim. Ital.*, 1962, **92**, 811 (*synth*)
Kolbin, N.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 1334; 1968, **13**, 479 (*synth, ir, props*)
Brodersen, K. *et al, J. Less-Common Met.*, 1968, **15**, 347 (*synth, struct*)

IC-001947

Br_3La
Lanthanum(*III*) bromide ($LaBr_3$)
Lanthanum tribromide
[13536-79-3]

$LaBr_3$

M 378.6
Has the UCl_3 struct. in solid state, pyramidal in gas phase. White solid. Sol. H_2O, Py, DMF; sl. sol. THF, MeCN. Mp 783°.
Heptahydrate: [13465-19-5].
$Br_3H_{14}LaO_7$ M 504.7
Colourless cryst. Sol. H_2O, EtOH. Prob. isostructural with corresp. chloride.

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*cryst struct*)
Richman, I. *et al, J. Chem. Phys.*, 1963, **39**, 1833 (*raman*)
Mayer, I. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*heptahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Asawa, C.K., *Phys. Rev.*, 1968, **173**, 869 (*raman*)
Dudchik, G.P. *et al, Zh. Fiz. Khim.*, 1975, **49**, 1856 (*ep*)
Berthou, H. *et al, Chem. Phys. Lett.*, 1976, **38**, 199 (*pe*)
Giricheva, N.I. *et al, CA*, 1977, **87**, 11948 (*ed*)

Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6**, 56 (*rev*)
Uwamino, Y. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al, J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

Br_3Lu IC-001948
Lutetium(*III*) bromide ($LuBr_3$)
Lutetium tribromide
[14456-53-2]

$LuBr_3$

M 414.6
White solid. Sol. H_2O, THF. Mp 1025° (960°). Bp ~1440°.
Hexahydrate: [15162-89-7].
$Br_3H_{12}LuO_6$ M 522.7
Colourless cryst. Sol. H_2O. Isostructural with corresp. chloride. Loses H_2O on controlled heating *in vacuo*.

Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6** (*rev*)
Mayer, I. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al, J. Chem. Soc. A*, 1968, 1889 (*hexahydrate, synth, cryst struct*)
Bastle, L.J. *et al, J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Giricheva, N.I. *et al, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1974, **17**, 616; *CA*, **81**, 42590 (*ed*)
Ruscic, B. *et al, Ann. Isr. Phys. Soc.*, 1984, **6**, 173 (*pe*)
Loktyushina, N.S. *et al, Zh. Fiz. Khim.*, 1984, **58**, 2631 (*ir*)
Uwamino, Y. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al, J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

$Br_3Mn^\ominus$ IC-001949
Tribromomanganate(*II*)(1−)
$[MnBr_3]^\ominus$

M 294.6 (ion)
K salt: Potassium tribromomanganate(III) (*$KMnBr_3$*). *Manganese*(III) *potassium bromide* (*$MnKBr_3$*)
Br_3KMn M 333.7
Synth. by heating a 1:1 mixt. of KBr and $MnBr_2$. Hygroscopic cryst. μ_{eff} = 5.67μ_B(293K). Struct. contains double chain -edge sharing $MnBr_6$ octahedra of NH_4CdCl_3 type.
Rb salt: [38669-02-2]. *Rubidium tribromomanganate*(II) (*$RbMnBr_3$*). *Manganese*(II) *rubidium bromide* (*$MnRbBr_3$*)
Br_3MnRb M 380.1
Synth. from $MnCO_3$ and aq. HBr and heating the product in an atm. of dry HBr gas. Mp 452°. Antiferromagnetic at low temps. Struct. contains face sharing $MnBr_6$ chains of $CsNiCl_3$ type.
Cs salt: [36482-50-5]. *Caesium tribromomanganate*(II) (*$CsMnBr_3$*). *Caesium manganese*(II) *bromide* (*$CsMnBr_3$*)
Br_3CsMn M 427.5
Synth. from Cs_2CO_3 and $MnCO_3$ and aq. HBr and heating the product in thepresence of dry HBr gas. Hygroscopic cryst. Mp 554° (565°). μ_{eff} = 4.90μ_B (293K). Antiferromagnetic at low temp.. Struct. contains facesharing $MnBr_6$ chains of $CsNiCl_3$ type.
Me_3NH salt: Synth. by heating a 1:1 mixt. of $[Me_3NH]Br$ and $MnBr_2$. Pink needles.
Me_4N salt: [51139-56-1].
Synth. by heating 1:1 mixt. of $[Me_4N]Br$ and $MnBr_2$. Pink needles. Struct. contains face sharing $MnBr_6$ chains of $CsNiCl_3$ type.
Et_4N salt: [51139-57-2].
Synth. by heating 1:1 mixt. of $[Et_4N]Br$ and $MnBr_2$.

Foster, J.J. *et al, J. Chem. Soc. A*, 1968, 2625 (*synth, str*)
Goodyear, J. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 1648 (*synth, struct*)
Seifert, H.J. *et al, Z. Anorg. Allg. Chem.*, 1972, **391**, 303 (*synth, struct, magnetism*)
McPherson, G.L. *et al, Inorg. Chem.*, 1973, **12**, 1196 (*synth, ir*)
McPherson, G.L. *et al, J. Chem. Phys.*, 1974, **60**, 104 (*magnetism*)
Pustik, C.F. *et al, Inorg. Chem.*, 1976, **15**, 272 (*ac-stc*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, **C5**, 299; 1983, **C10**, 47 (*rev, bibl, ac-stc*)
Crisp, J.R., *Coord. Chem. Rev.*, 1982, **45**, 237 (*struct*)

Br_3Mo IC-001950
Molybdenum bromide ($MoBr_3$), 9Cl
Molybdenum tribromide. Molybdic bromide
[13446-57-6]

$MoBr_3$

M 335.6
Prepd. by heating Mo in a stream of Br_2 at 350°. Dark green or black needles. Deliquescent. Insol. H_2O, EtOH.

Inorg. Synth., 1967, **10**, 40 (*synth*)
Boyd, P.D.W. *et al, Aust. J. Chem.*, 1969, **22**, 2595 (*str*)
Druce, P.M. *et al, J. Chem. Soc. A*, 1971, 3595 (*synth, anhyd*)
Babel, D., *J. Solid State Chem.*, 1972, **4**, 403 (*cryst struct*)
Oppermann, H., *Z. Anorg. Allg. Chem.*, 1973, **395**, 249 (*thermodyn*)

Br_3MoN IC-001951
Molybdenum(*VI*) bromide nitride ($MoBr_3N$), 9Cl
[68926-06-2]

$MoBr_3N$

M 349.6
Prepd. from $MoBr_4$ + IN_3 in CCl_4 suspension. V. hygroscopic brown powder. Ir spectrum agrees with an Mo—N triple bond.

Dehnicke, K. *et al, Z. Naturforsch., B*, 1978, **33**, 1242 (*synth, ir*)

Br_3MoN_3 IC-001952
Molybdenum(*IV*) azide bromide ($Mo(N_3)Br_3$), 9Cl
Molybdenum(IV) *bromide nitride* (*$MoBr_3N_3$*)
[68825-98-9]

$Mo(N_3)Br_3$

M 377.6
Prepd. from $MoBr_4$ + IN_3. Dark brown, hygroscopic powder.
▷ Explosive in the dry state.

Dehnicke, K. *et al, Z. Naturforsch., B*, 1978, **33**, 1242 (*synth, ir*)

Br_3MoO IC-001953
Molybdenum(*V*) bromide oxide ($MoBr_3O$), 9Cl
Molybdenum(V) *oxytribromide*
[13596-04-8]

$MoOBr_3$

M 351.6
Prepd. from MoO_2Br_2 + PBr_5 or from 'moist' $MoBr_3$ + Br_2 under reflux. Grey-black solid. Insol. H_2O.

Colton, R. *et al, Aust. J. Chem.*, 1965, **18**, 447 (*synth*)
Crouch, P.C. *et al, J. Chem. Soc. A*, 1968, 1061 (*synth, ir*)
Drew, M.G.B. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 1161 (*cryst struct*)
Oppermann, H. *et al, Z. Anorg. Allg. Chem.*, 1972, **387**, 339 (*thermodyn*)

Br_3N IC-001954

Nitrogen tribromide

Tribromoamine. Nitrogen bromide (NBr_3)

[15162-90-0]

NBr_3

M 253.7

Synth. from Br_2 + NH_3 at −70°. Fairly stable in dil. aq. solns. if excess Br_2 is present. Sol. H_2O. v. sol. $CHCl_3$. λ_{max} 260 nm.

▷ Explosive even at −100°.

Jander, J. *et al*, *Z. Anorg. Allg. Chem.*, 1966, **349**, 57 (*synth*)
Jander, J., *Adv. Inorg. Chem. Radiochem.*, 1976, **19**, 2 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 244.
Soulard, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 2300 (*anal, equilibria in soln*)

Br_3NW IC-001955

Tungsten(*V*) bromide nitride (WBr_3N)

[76537-91-2]

$N{\equiv}WBr_3$

M 437.5

The *ir* spectrum indicates the presence of a W≡N triple bond. Synth. from IN_3 + WBr_5 or WBr_6 + $[Hg_2N]Br$ in CH_2Cl_2 at 80°. Moisture-sensitive black powder.

Ruschke, P. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1589 (*synth, ir*)
Godemeyer, T. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **566**, 77 (*synth*)

Br_3Nb IC-001956

Niobium bromide ($NbBr_3$), 11CI

Niobium tribromide

[15752-41-7]

$NbBr_3$

M 332.6

Homogeneous phases exist with Br:Nb ratio between 2.67 and 3.03:1. See also Niobium bromide (Nb_3Br_8), IC-002214. Synth. from $NbBr_5$ and Nb at 400-500° or by H_2 reduction of $NbBr_5$. Dark brown solid. Subl. 400 *in vacuo*. Paramagnetic, μ_{eff} = $1.14\mu_B$, θ −140K.

Brubaker, C.H. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 4179 (*synth*)
Schaefer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1959, **300**, 1; 1961, **311**, 134 (*synth, phases*)
Berdonosov, S.S. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 1525 (*synth*)
Krylov, E.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1966, **11**, 541 (*magnetism*)

Br_3NbO IC-001957

Niobium(*V*) bromide oxide ($NbBr_3O$), 11CI

Niobium tribromide oxide

[14459-75-7]

$NbOBr_3$

M 348.6

Synth. by heating $NbBr_5$ with Nb_2O_5 or O_2 above 250°; or from Nb_2O_5 and BBr_3 at 280°. Yellow solid. Subl. $_{0.05}$ 190°.

Canterford, J.H. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 471 (*ir*)
Schultz, C.O. *et al*, *J. Phys. Chem.*, 1968, **72**, 4686 (*synth, ir*)
Dymo, P.M. *et al*, *J. Chem. Soc. A*, 1971, 3593 (*synth, ir*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1457 (*synth*)
Nunzianti-Cesaro, S. *et al*, *Spectrochim. Acta, Part A*, 1984, **40**, 579 (*ir*)

Br_3NbS IC-001958

Niobium(*V*) bromide sulfide ($NbBr_3S$), 11CI

Niobium tribromide sulfide

[60994-02-7]

$NbSBr_3$

M 364.6

Synth. from $NbBr_3$ and Sb_2S_3 in CS_2. Red solid.

Fowles, G.W.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1976, 552 (*synth*)
bin Baba, I., *Sains Malays.*, 1981, **10**, 69 (*synth*)
Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2251 (*reactions*)

Br_3NbSe IC-001959

Niobium(*V*) bromide selenide ($NbBr_3Se$), 11CI

Niobium tribromide selenide

[60994-04-9]

$NbSeBr_3$

M 411.5

Synth. from $NbBr_5$ and Sb_2Se_3 in CS_2 or in the solid state. Dark brown solid.

Fowles, G.W.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1976, 552 (*synth*)
bin Baba, I., *Sains Malays.*, 1981, **10**, 69 (*synth*)
Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 1087 (*synth, reactions*)

$Br_3Nb_3Se_{10}$ IC-001960

Niobium bromide diselenide ($Nb_3Br_3(Se_2)_6$), 11CI

Niobium bromide selenide ($Nb_6Br_6Se_{20}$)

[102402-06-2]

$Nb_3Br_3(Se_2)_5$

M 1308.0

Chain struct. in which one Nb is in sq. antiprismatic coordination by four Se_2 groups forming a bridge between two other Nb with 1 terminal Br and 1 bridging Se_2. Formed as a by-product in the synthesis of $NbSe_3Br$ from Nb + Se + Br_2 in a sealed SiO_2 tube at 600-700°. Black solid.

Meerschaut, A. *et al*, *J. Solid State Chem.*, 1986, **61**, 90 (*synth, cryst struct*)

Br_3Nd IC-001961

Neodymium(*III*) bromide ($NdBr_3$)

Neodymium tribromide

[13536-80-6]

$NdBr_3$

M 383.9

Has $PuBr_3$ struct. Green cryst. Sol. H_2O. Mp 684° (671°). Bp 1540°.

Hexahydrate: [29843-90-1].
$Br_3H_{12}NdO_6$ M 492.0
Blue cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Isostructural with corresp. chloride.

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265.

Meyer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, spa*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*hexahydrate, synth, cryst struct, ir*)
Basile, L.J. *et al*, *J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, C6, 61 (*rev*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)
Wilmarth, W.R. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 245 (*raman*)

Br_3NdO_9 IC-001962

Neodymium(*III*) bromate ($Nd(BrO_3)_3$)

Neodymium tribromate

$Nd(BrO_3)_3$

M 527.9

Nonahydrate: Nonaaquaneodymium(3+) tris(bromate)
$Br_3H_{18}NdO_{18}$ M 690.0
Red cryst. Insol. H_2O. Mp 66-67°. Contains tricapped trigonal prismatic $Nd(OH_2)_9^{3\oplus}$ ions. Loses H_2O at 150°.

Helmholz, L., *J. Am. Chem. Soc.*, 1939, **61**, 1544.

$Br_3Ni^{\ominus}$ IC-001963

Tribromonickelate(*II*)(1−), 8CI

$[NiBr_3]^{\ominus}$

M 298.4 (ion)

Octahedral polymer. Antiferromagnetic. Many studies of magnetism, uv-vis spectra etc at low temps. particularly of Cs salt.

Cs salt: [15455-70-6]. *Caesium nickel bromide ($CsNiBr_3$)*
Br_3CsNi M 431.3
Brown cryst.

Me_4N salt: [15455-68-2].
Red brown needles.

[65621-37-6]

Asmussen, R.W. *et al*, *Z. Anorg. Allg. Chem.*, 1956, **283**, 3 (*synth*)
Stucky, G.D. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 4828 (*synth, cryst struct*)
McPherson, G.L. *et al*, *Inorg. Chem.*, 1973, **12**, 1196 (*synth, ir*)
Dupas, C. *et al*, *J. Chem. Phys.*, 1974, **61**, 3871 (*magnetism*)
Brener, R. *et al*, *J. Phys. Chem. Solids*, 1977, **38**, 1023 (*magnetism, Cs-133 nmr*)
Reber, C. *et al*, *Inorg. Chem.*, 1986, **25**, 1196 (*uv-vis, fluorescence*)

Br_3Np IC-001964

Neptunium(*III*) bromide ($NpBr_3$)

Neptunium tribromide

[20730-39-6]

$NpBr_3$

M 476.7

Exists in α (hexagonal) and β (orthorhombic)forms. α-form has UCl_3 structure (9-coordinate). β-form has $PuBr_3$ structure (8-coordinate). Green solid. Sol. H_2O. Subl. 800°. μ_{eff} = $3.26\mu_B$ (50-125K).

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*struct*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1757 (*synth, struct*)
Jones, E.R. *et al*, *J. Chem. Phys.*, 1974, **60**, 2088 (*magnetism*)
Carnall, W.T. *et al*, *J. Chem. Phys.*, 1974, **61**, 4993 (*synth, uv-vis*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1268 (*synth*)

Br_3OP IC-001965

Phosphoryl bromide, 9CI, 8CI

Tribromophosphine oxide. Tribromooxophosphorus(V). Phosphorus tribromide oxide. Phosphorus(V) bromide oxide (PBr_3O)

[7789-59-5]

$P(O)Br_3$

M 286.6

Interatomic distances (vap.): P═O 145.5, P—Br 217.5 pm; angles: OPBr 114.4°, BrPBr 104.1° Synth. from PBr_5 + P_4O_{10} at 150°. Brominating agent and phosphorylating agent. Large flaky cryst. Yellows and dec. at high temps. Slowly dec. by $H_2O \rightarrow H_3PO_4$ + HBr. Sol. org. solvs. Mp 55°. Bp 193°, Bp_{20} 125°. ΔH_f° −386 kJ mol^{-1}.

▷ Poison, corrosive, irritant. TH4750000.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 506 (*rev, bibl*)
Lappert, M.F. *et al*, *J. Chem. Soc. A*, 1967, 129 (*synth*)
Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **354**, 139 (*P-31 nmr*)
Olie, K. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 974 (*cryst struct*)
Templeton, L. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 1678 (*cryst struct*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 524, 1153 (*rev*)
Haler, E. *et al*, *J. Mol. Struct.*, 1972, **12**, 121 (*ir, raman, cryst struct*)
Olie, K. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1973, **92**, 751 (*ir, raman, cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 520, 534 (*synth*)
Grossmann, G. *et al*, *Z. Chem.*, 1976, **16**, 362 (*O-17 nmr*)
Jacob, E.J. *et al*, *J. Mol. Struct.*, 1980, **62**, 143 (*ed, struct*)
Binnewies, M. *et al*, *Thermochim. Acta*, 1986, **103**, 401 (*mu*)
Nyquist, R.A., *Appl. Spectrosc.*, 1987, **41**, 272 (*ir, raman*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2781.

Br_3OPa IC-001966

Protactinium bromide oxide ($PaBr_3O$)

Tribromooxoprotactinium(V). μ-Bromodibromo-μ_5-oxoprotactinium(V). Protactinium tribromide oxide

[15608-27-2]

$PaOBr_3$

M 486.7

Pentagonal bipyramidal Pa, bound to 4Br and 3O in double-chain struct. Yellow monoclinic cryst.

Brown, D. *et al*, *Nature (London)*, 1968, **217**, 737 (*cryst struct*)
Brown, D. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1382 (*synth*)

Br_3OTa IC-001987

Tantalum(*V*) bromide oxide ($TaBr_3O$), 11CI

Tantalum oxytribromide

[15608-28-3]

$TaOBr_3$

M 436.6

Synth. by passing O_2 over $TaBr_5$ at 200° or less satisfactorily by pyrolysing a $TaBr_5/Et_2O$ complex or heating Ta_2O_5 + CBr_4. Used in diene polym. catalysts. Yellow, thermally unstable solid.

Chaigneau, M., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **248**, 3173 (*synth*)
Fairbrother, F. *et al*, *J. Less-Common Met.*, 1959, **1**, 206 (*synth*)
Netherlands Pat., 297 866, (1965); *CA*, **64**, 11424g (*use*)
Dittmer, G. *et al*, *Philips J. Res.*, 1985, **40**, 55 (*thermodyn*)

Br_3OU IC-001968

Tribromooxouranium(*V*)

Uranium(V) *bromide oxide* (UBr_3O). *Uranium tribromide oxide*

[14853-40-8]

$UOBr_3$

M 493.7

7-Coord., isostructural with $PaOBr_3$. Synth. from UO_3 + CBr_4/N_2 (110°). Affords $UOBr_2$ at >200°. Moisture-sensitive brown solid. Thermally unstable at r.t., slowly evolves Br_2. Sol. $CHCl_3$, dec. by Me_2CO, EtOH.

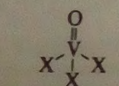
Prigent, J., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1953, **236**, 710; 1954, **239**, 424.
Shchukareva, S.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1958, **3**, 75.
Kaufman, G. *et al*, *Bull. Soc. Chim. Fr.*, 1961, 1969.
Kaufman, G., *Rev. Chim. Minér.*, 1964, **1**, 129.
Prigent, J., *Ann. Chim.* (*Paris*), 1965, **5**, 65.

Br_3OV IC-001969

Vanadium bromide oxide (VBr_3O)

Vanadium oxide tribromide. Tribromooxovanadium(V), *IICI. Oxytribromovanadium*(V)

[13520-90-6]



C_{3v}

X = Br

M 306.6

Synth. by reaction of V_2O_5 + C + Br_2 at 200° in a flow system. Astringent for antiperspirants. Deep-red liq.; hydrol. in air; dec. slowly at r.t. Sol. CH_2Br_2. Mp −59°. Bp 170°.

▷ Reacts violently with H_2O.

Miller, F.A. *et al*, *Spectrochim. Acta*, 1961, **17**, 112 (*synth, ir*)
Clark, R.J.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1971, 2429 (*raman*)
Mueller, U. *et al*, *Z. Naturforsch., B*, 1982, **37**, 699 (*reaction*)
Natarajan, A. *et al*, *Indian J. Phys., B*, 1983, **57**, 234 (*ir, raman*)
U.S. Pat., 4 490 354, (1984); *CA*, **102**, 100626b (*use*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3457 (*haz*)

Br_3OW IC-001970

Tungsten(*V*) bromide oxide (WBr_3O)

Tunsten oxytribromide

[20213-56-3]

$WOBr_3$

M 439.5

Prepd. by heating stoichiometric amounts of W, WO_3 and Br_2; by reduction of $WOBr_4$ with Al powder; and by reaction of WBr_5 with Sb_2O_3. Blue-black needles. Stable in air.

Tillack, J. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1968, **7**, 294 (*synth*)
Crouch, P.C. *et al*, *J. Chem. Soc. A*, 1968, 1061; 1969, 2412 (*synth, cryst struct*)
Oppermann, H. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **387**, 329 (*thermodyn*)
Inorg. Synth., 1973, **14**, 109 (*synth*)

Br_3O_9Pr IC-001971

Praseodymium(*III*) bromate ($Pr(BrO_3)_3$)

$Pr(BrO_3)_3$

M 524.6

Green cryst. V. sol. H_2O.

Nonahydrate: [63427-20-3]. *Nonaaquapraseodymium*(3+) *tris*(*bromate*)
$Br_3H_{18}O_{18}Pr$ M 686.7
Green cryst. Sol. H_2O. Mp 56.5°. Isomorphous with other lanthanide bromates; contains tricapped trigonal prismatic $Pr(OH_2)_9^{3\oplus}$ ions. Dec. >50° (H_2O lost); >250°, Br_2, O_2, PrOBr formed.

James, C. *et al*, *J. Am. Chem. Soc.*, 1908, **30**, 182; 1909, **31**, 913 (*synth*)
Bancroft, G.H. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1545.
Staveley, L.A.K. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
Poulet, H. *et al*, *Phys. Status Solidi A*, 1975, **32**, 509 (*ir, raman*)
Albertsson, J. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1460 (*synth, cryst struct*)

Br_3O_9Sm IC-001972

Samarium(*III*) bromate ($Sm(BrO_3)_3$)

[28958-26-1]

$Sm(BrO_3)_3$

M 534.0

Nonahydrate: [63427-22-5]. *Nonaaquasamarium*(3+) *tris*(*bromate*)
$Br_3H_{18}O_{18}Sm$ M 696.2
Pink hexagonal cryst. V. sol. H_2O; sl. sol. EtOH. Mp 75°. Loses H_2O >150°. Contains $Sm(OH_2)_9^{3\oplus}$ ions.

Spedding, F.H. *et al*, *Phys. Rev.*, 1933, **44**, 287 (*synth*)
Kremers, H.E. *et al*, *J. Am. Chem. Soc.*, 1944, **66**, 1795 (*synth*)
Stavely, L.A.K. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
Sikka, Z.K., *Acta Crystallogr., Sect. A*, 1969, **25**, 621 (*cryst struct*)
Poulet, H. *et al*, *Phys. Status Solidi A*, 1975, **32**, 509 (*ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. vol.*, 1978, **C6**, 93 (*rev*)

Br_3O_9Y IC-001973

Yttrium(*III*) bromate ($Y(BrO_3)_3$)

[15162-95-5]

$Y(BrO_3)_3$

M 472.6

Nonahydrate: Nonaaquayttrium(3+) *tris*(*bromate*)
$Br_3H_{18}O_{18}Y$ M 634.7
Colourless prisms. V. sol. H_2O, sl. sol. EtOH. Mp 74°. Loses $6H_2O$ at 100°.

Kremers, H.E. *et al*, *J. Am. Chem. Soc.*, 1944, **66**, 1795 (*synth*)
Albertsson, J. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1460 (*cryst struct*)

Br_3Os IC-001974

Osmium(*III*) bromide ($OsBr_3$)

Osmium tribromide

[59201-51-3]

$OsBr_3$

M 429.9

The existence of $OsBr_3$ has not yet been proven. Synth. by thermal dec. of $OsBr_4$ or by heating 'Os_2Br_9' at 350 to 400° in sealed tube. Catalyst for hydroxylation of

alkenes. Dark grey powder. Insol. H_2O, org solvs, mineral acids. Mp 340° dec. Calculated ΔH_f° −97.8 kJ mol^{-1}. Dec. to the elements upon heating to 340° *in vacuo*.

Schukarev, S.A. *et al*, *Zh. Neorg. Khim.*, 1961, **6**, 1246; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1961, **6**, 638 (*synth, props*)
Burylev, B.P., *Zh. Fiz. Khim.*, 1975, **49**, 2671; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1975, **49**, 1568 (*props*)
U.S. Pat., 4 496 778, (1985); *CA*, **102**, 148723h (*use*)
Thiele, G. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **530**, 178 (*ed*)
Schefer, H., *Z. Anorg. Allg. Chem.*, 1986, **535**, 219 (*struct*)

Br_3P IC-001975

Phosphorus bromide (PBr_3)

Phosphorous tribromide, 9CI. Tribromophosphine. Phosphorous tribromide(III)

[7789-60-8]

PBr_3

M 270.6

Orthorhombic at low temps., having interatomic distance: P—Br 222.0 pm; angle: BrPBr 101.0°. Synth. from P + Br_2 in PBr_3. Brominating agent. Used for conversion of alcohols into alkyl bromides. Colourless fuming liq. V. reactive to protic nucleophiles. d_4^{20} 2.87, d_4^0 2.92. Mp −41.5°. Bp 173°. Forms stable adducts with boron trihalides. ΔH_f° −125 kJ mol^{-1}.

▷ Reacts violently with H_2O. Corrosive. TH4460000.

BBr_3 complex (1:1): see *Tribromo*(*phosphorous tribromide*) *boron, IC-000783*

BI_3 complex (1:1):
BBr_3I_3P M 662.2
Solid. Mp 50° dec.

Inorg. Synth., 1946, **2**, 147 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 17, 1965, C, 491 (*rev, bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 873; 1980, **8**, 400 (*uses*)
Kuchitsu, K. *et al*, *Inorg. Chem.*, 1971, **10**, 2584 (*ed, microwave, struct*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 518, 1143 (*rev*)
Varmuza, K. *et al*, *Monatsh. Chem.*, 1971, **102**, 1037 (*ms*)
Betteridge, D. *et al*, *Anal. Chem.*, 1972, **44**, 2005 (*pe*)
Daamen, H. *et al*, *Inorg. Chim. Acta*, 1978, **28**, 263 (*pe*)
Enjalbert, R. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 546 (*cryst struct*)
Van Linthaudt, J.P. *et al*, *Spectrochim. Acta, Part A*, 1979, **35**, 1307 (*P-31 nmr*)
Van Lindhaudt, J.P. *et al*, *J. Mol. Struct.*, 1980, **67**, 269 (*struct*)
Buckingham, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1167 (*P-31 nmr*)
Nyquist, R.A. *et al*, *Appl. Spectrosc.*, 1987, **41**, 272 (*ir, raman*)
Mikov, S.N. *et al*, *Zh. Prikl. Spektrosk.*, 1987, **47**, 765; *Soviet J. Appl. Spectrosc.*, 1987, **47**, 1140 (*raman*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2780 (*haz*)

Br_3PS IC-001976

Thiophosphoryl bromide, 9CI

Tribromophosphine sulfide. Phosphorus sulfobromide. Tribromosulfophosphine. Phosphorus tribromide sulfide. Tribromothioxophosphorus(V). *Phosphorus*(V) *bromide sulfide* (*PBr_3S*)

[3931-89-3]

$P(S)Br_3$

M 302.7

Interatomic distances (vap.): P=S 189.5, P—Br 219.3 pm; angles: SPBr 116.2°, BrPBr 101.9°. Synth. from PBr_5 + P_4S_{10} at 100°. Thiophosphorylating agent. Yellow, regular octahedral cryst. (CS_2/pet ether). Fairly stable to H_2O. Readily sol. Et_2O, CS_2, $CHCl_3$. Mp 38°. Bp 212-215° dec.; Bp_{25} 125-130°. Over Ag at 800° → Phosphenothious bromide, IC-001748.

▷ Pungent vapour. Mod. toxic. Can produce corrosive, toxic fumes with H_2O or steam.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 599 (*rev, bibl*)
Müller, A. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1967, **71**, 571 (*ir, raman*)
Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **354**, 139 (*P-31 nmr*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 546, 1153 (*rev*)
Cox, P.A. *et al*, *Faraday Discuss. Chem. Soc.*, 1972, No. 54, 26 (*pe*)
Olie, K. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1973, **92**, 751 (*ir, raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 521 (*synth*)
Jacob, E.J. *et al*, *J. Mol. Struct.*, 1980, **62**, 143 (*ed*)
Nyquist, R.A., *Appl. Spectrosc.*, 1987, **41**, 272 (*ir, raman*)
Binnewies, M. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **552**, 147 (*props*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3261.

Br_3PSe IC-001977

Selenophosphoryl bromide, 10CI

Tribromophosphine selenide. Tribromoselenoxophosphorus(V). *Phosphorus*(V) *bromide selenide* (*PBr_3Se*)

[62565-69-9]

$P(Se)Br_3$

M 349.6

Not isol. Synth. from PBr_3 + Se or from $MeSePBr_2$ + Br_2. Phys. props. not recorded.

Baudler, M. *et al*, *Z. Naturforsch., B*, 1977, **32**, 347 (*synth, P-31 nmr*)

Br_3Pm IC-001978

Promethium(*III*) bromide ($PmBr_3$)

Promethium tribromide

[14325-78-1]

$PmBr_3$

M 384.6

8-Coord.; adopts the $PuBr_3$ struct. Coral-red cryst. Sol. H_2O. Mp 660° (est.), (625°).

[116797-91-2]

Weigel, F. *et al*, *Radiochim. Acta*, 1967, **7**, 40 (*synth, cryst struct*)
Wishnevsky, V. *et al*, *J. Less-Common Met.*, 1984, **99**, 321 (*hydrol, thermodyn*)
Wilinarth, W.R. *et al*, *J. Less-Common Met.*, 1988, **141**, 275 (*raman, struct*)
Wilinarth, W.R. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 271 (*raman, struct*)

Br_3Pr IC-001979

Praseodymium(*III*) bromide ($PrBr_3$)

Praseodymium tribromide

[13536-53-3]

$PrBr_3$

M 380.6

Has UCl_3 struct. Green cryst. Sol. H_2O, THF. Mp 693° (691°). Bp 1547°.

Heptahydrate: [20736-90-7].
$Br_3H_{14}O_7Pr$ M 506.7
Green cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Prob. isostructural with corresp. chloride.

Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*struct*)
Mayer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*heptahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*ir*)
Basile, L.J. *et al*, *J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, **C6**, 59 (*rev*)
Chivian, J.S. *et al*, *J. Opt. Soc. Am.*, 1979, **69**, 1622 (*ir, vis*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

Br_3Pt IC-001980

Platinum(*III*) bromide ($PtBr_3$), 9CI
Platinum tribromide
[25985-07-3]

$PtBr_3$

M 434.7
Struct. contains Pt_6Br_{12} octahedra (see Platinum(*II*) bromide ($PtBr_2$), IC-001880) and chains of $PtBr_6$ octahedra. Synth. from Platinum(*IV*) bromide ($PtBr_4$), IC-002067 heated in Br_2 (g). Green-black solid.

Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1607.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1714 (*synth*)
Wells, A.F., *Structural Inorg. Chem.*, 5th Ed., Oxford, 1984, 423 (*struct*)

Br_3Pu IC-001981

Plutonium(*III*) bromide ($PuBr_3$)
Plutonium tribromide
[15752-46-2]

$PuBr_3$

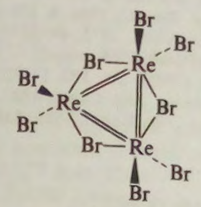
M 478.7
Structural prototype. 8-Coord. Pu in layer struct. with layer packing unusually close for contact between non-bonded Br atoms. Light green solid. Sol. H_2O. Mp 681°. Reacts with water to form hexahydrate.

Hexahydrate: [20737-00-2].
Hexaaquadibromoplutonium(1+) bromide
Blue cryst. Sol. H_2O. Can be dehydrated to $PuBr_3$ on careful heating *in vacuo* at 70-120°. Probably best formulated as $PuBr_2(OH_2)_6^{\oplus}Br^{\ominus}$.

Fomin, V.V. *et al*, *Zh. Neorg. Khim.*, 1958, **3**, 2231.
Lipis, L.V. *et al*, *Zh. Neorg. Khim.*, 1960, **5**, 2162; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1960, **5**, 1049 (*uv-vis*)
Gruen, D.M. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 2569 (*uv-vis*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*synth, ir, cryst struct, hexahydrate*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1757 (*cryst struct*)
Jones, E.R. *et al*, *J. Chem. Phys.*, 1974, **60**, 2088 (*magnetism*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1302 (*synth*)
Weigel, F. *et al*, *J. Less-Common Met.*, 1982, **84**, 141 (*synth*)

Br_3Re IC-001982

Rhenium(*III*) bromide ($ReBr_3$), 9CI
Rhenium tribromide
[13569-49-8]



trimer

M 425.9
Trimeric; detailed molecular geometry not determined. Synth. (i) from $Re_2(OAc)_4Cl_2$ and HBr at 340° for 3 hrs., (ii) by thermal dec. of Ag_2ReBr_6 or $ReBr_5$, (iii) from Re and Br_2. Lustrous black cryst. Pale yellow-green vapour at 430°. Sol. Me_2CO, MeOH, EtOH, HBr aq. Subl. 500°.

Trimer: [33517-16-7]. *Tri-μ-bromohexabromotrirhenium*(III), *9CI*
Br_9Re_3 M 1277.7

Hagan, H. *et al*, *Z. Anorg. Allg. Chem.*, 1933, **215**, 111 (*synth, props*)
Colton, R., *J. Chem. Soc.*, 1962, 2072 (*synth, props*)
Inorg. Synth., 1967, **10**, 58; 1980, **20**, 47 (*synth, props*)
Cotton, F.A., *Multiple Bonds Between Metal Atoms*, Wiley, New York, 1982, 267 (*struct*)

Br_3Rh IC-001983

Rhodium(*III*) bromide ($RhBr_3$), 8CI
Rhodium tribromide. Tribromorhodium
[15608-29-4]

$RhBr_3$

M 342.6
Prepared by heating Rh metal in a 45% HBr-Br_2 mixture, then treating the product in a Br_2 stream at 400°. Commercially available. Dark brown plates. Insol. acids, org. solvs. Thermally stable up to 805° at which temp. dec. commences. Insolubility restricts synthetic use.

Thiele, G., *Fortschr. Chem. Forsch.*, 1968, **10**, 631, 644.
Brodersen, K., *J. Less-Common Met.*, 1968, **14**, 151 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1739 (*synth*)

Br_3Ru IC-001984

Ruthenium(*III*) bromide ($RuBr_3$)
Ruthenium tribromide
[14014-88-1]

$RuBr_3$

M 340.7
Exists as chains of $(Ru_2Br_3)Br_{\frac{6}{2}}$ groups, with the metal in approx. octahedral coordination. The short Ru—Ru distance between discrete Ru_2 pairs is 273 pm; the Ru_2 units are separated by 312 pm. Ru—Br 246 (within dimeric units); Ru—Br 253 pm (between units). Prepd. by direct combination of the elements at 450-500°/20 atm. Black rhombic cryst. Insol. H_2O, acid, EtOH and other common solvs. Dec. >500° to give Ru + Br_2. Shows weak temp.-independent paramagnetism. ΔG_f° −126 kJ mol^{-1}. ΔH_f° −184 kJ mol,$^{-1}$. ΔS° −205 J K^{-1} mol^{-1}.

Hydrated-form
Ruthenium(III) *bromide* (*hydrated*). *Soluble ruthenium*(III) *bromide*
$RuBr_3.xH_2O$. Like commercial ruthenium(*III*) chloride, this material is prob. a heterogenous mixt. of bromide, oxide bromide and aquabromo complexes. Prepd. by adding RuO_4 to aq. HBr or by dissolving 'ruthenium(*III*) hydroxide' in aq. HBr. V. useful starting material for the synth. of bromide complexes. Red-brown solid. V. sol. H_2O, HBr.

Gutbier, A. *et al*, *Z. Anorg. Allg. Chem.*, 1905, **45**, 166; 1919, **109**, 187 (*hydrated-form, synth*)
Krauss, F. *et al*, *Z. Anorg. Allg. Chem.*, 1924, **137**, 32 (*hydrated-form, synth*)
Shchukarev, S.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1960, **5**, 923 (*synth, thermal dec.*)
Shchukarev, S.A. *et al*, *Vestn. Leningrad Univ. Ser. Mat. Fiz. Chem.*, 1961, **16**, 100 (*synth, thermodynamics*)
Brodersen, K., *Angew. Chem., Int. Ed. Engl.*, 1968, **7**, 147, 148 (*cryst struct*)
Brodersen, K. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **357**, 162 (*cryst struct, magnetism*)
Kaindl, G. *et al*, *Z. Phys. Chem. (Leipzig)*, 1969, **226**, 103 (*mössbauer*)
Clausen, C.A. *et al*, *Chem. Phys. Lett.*, 1971, **8**, 565 (*mössbauer*)
Appleby, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1990, 1879 (*hydrated-form, synth*)

Br_3STa IC-001985

Tantalum(*V*) bromide sulfide ($TaBr_3S$), 11CI
[60994-05-0]

$TaBr_3S$

M 452.7
Synth. from $TaBr_5$ and Sb_2S_3 in CS_2 in the absence of O_2 or from $TaBr_5$ and Sb_2S_3 at 110° for 10 days. Red-orange solid. Forms adducts $TaBr_3SL_2$(L = MeCN, tetrahydrothiophene, Me_2S).

bin Baba, I., *Sains Malays.*, 1981, **10**, 29 (*synth, ir*)
Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 845 (*synth, complexes*)

Br_3Sb IC-001986

Antimony(*III*) bromide ($SbBr_3$), 8CI
Tribromostibine, 9CI. Tribromoantimony(III). *Antimonous bromide*
[7789-61-9]

$SbBr_3$

M 361.4
Synth. from Sb + Br_2; $SbCl_3$ or Sb_2O_3 + BBr_3. White cryst. becoming amber yellow when fused. Hygroscopic. Sol. H_2O. Sol. dil. HCl, HBr, CS_2, Me_2CO, C_6H_6, $CHCl_3$. Mp 96°. Bp 288°, Bp_2 135°. A Lewis acid, forming adducts with Lewis bases e.g. aromatic hydrocarbons; NH_3, amines. Reactive to O, N and S nucleophilic reagents, as well as carbanionic reagents e.g. alkyl(aryl)lithiums and Grignard reagents. ΔH_f° −259 kJ mol^{-1}. Forms complex bromides with bromides of other metals e.g. those of Group I. Dec. in H_2O, light, EtOH.

▷ Poison. Corrosive, can cause severe burns. CC4400000.

Benzene complex (*2:1*): (*Benzene*)*bis*[*tribromoantimony*(III)]
$C_6H_6Br_6Sb_2$ M 801.0
Monoclinic cryst. Mp 93°.
Mesitylene complex (*1:1*): [35075-49-1]. *Tribromo*(*1,3,5-trimethylbenzene*)*antimony*(III)
$C_9H_{12}Br_3Sb$ M 481.6
Trigonal. Colourless cryst. Mp 56-58°.
Hexamethylbenzene complex (*2:1*): [110296-09-8]. (*Hexamethylbenzene*)*bis*[*tribromoantimony*(III)]
$C_{12}H_{18}Br_6Sb_2$ M 885.1
Tetragonal colourless cryst. Mp 145°.
Biphenyl complex (*2:1*): [15068-72-1]. (*Biphenyl*) *bis*[*tribromoantimony*(III)]
$C_{12}H_{10}Br_6Sb_2$ M 877.1
Cryst. Mp 60.5°.
9,10-Dihydroanthracene complex (*2:1*): [122213-21-2]. $[\eta^2,(\eta^6)'$-*9,10-Dihydroanthracene*] *bis*[*tribromoantimony*(III)]
$C_{14}H_{12}Br_6Sb_2$ M 903.1
V. hygroscopic, colourless cryst. Stable under N_2. Mp 95-96°.

α-form
Discrete pyramidal molecules. Orthorhombic. Interatomic distances: Sb—Br 250 pm; angle BrSbBr 95.5°. Mp 96°.

β-form
Orthorhombic. Interatomic distances: Sb—Br 249 pm (mean), BrSbBr 95.1° (mean). V. hygroscopic needles (warm CS_2). Mp 96°.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1929, **9**, 493 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 18, 1949, 471 (*rev, bibl*)
Cushen, D.W. *et al*, *J. Chem. Soc.*, 1962, 2218; 1964, 4162 (*cryst struct*)
Lappert, M.F. *et al*, *J. Chem. Soc. A*, 1967, 129 (*synth*)
Okuda, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 2398 (*complex, cryst struct*)
Semin, G.K., *Phys. Status Solidi A*, 1972, **11**, K61 (*nqr*)
Lee, T.H. *et al*, *J. Chem. Phys.*, 1974, **60**, 1172 (*pe*)
Bowen, L.H. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 101 (*complexes, mössbauer*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 591 (*synth*)
Kjuntsel, I.A. *et al*, *J. Mol. Struct.*, 1982, **83**, 357 (*mössbauer, complexes*)
Lipka, A. *et al*, *Z. Naturforsch., B*, 1982, **37**, 695 (*complexes, cryst struct*)
Grodzicki, M. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1319 (*pe*)
Schmidbaur, H. *et al*, *Chem. Ber.*, 1987, **120**, 1829, 1837 (*complexes, cryst struct*)
Merck Index, 11th Ed., 1989, 738 (*props*)
Schmidbaur, H. *et al*, *Chem. Ber.*, 1990, **123**, 19 (*complex, cryst struct*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 284.

Br_3Sc IC-001987

Scandium(*III*) bromide ($ScBr_3$)
Scandium tribromide
[13465-59-3]

$ScBr_3$

M 284.6
Possesses the BiI_3 ($FeCl_3$) struct. Synth. from Sc_2O_3/HBr/NH_4Br followed by sublimation; or from $ScH_{1.7}$ + Br_2 at 500°. White cryst. Sol. H_2O. Mp 970° (948°). Subl. 800° *in vacuo*.

Hexahydrate: [20662-15-1]. *Scandium*(III) *bromide hexahydrate*
$Br_3H_{12}O_6Sc$ M 392.7
Deliquescent rhombic colourless cryst. Sol. H_2O. Loses H_2O >110°, dec. at 175°. Probably $[Sc(OH_2)_6]^{3\oplus}3Br^{\ominus}$.

Crookes, W., *Philos. Trans. R. Soc. London, A*, 1908, **209**, 15; 1910, **210**, 359 (*synth*)
Menkov, A.A. *et al*, *Zh. Neorg. Khim.*, 1964, **9**, 1759; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 952 (*synth, cryst struct*)

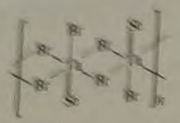
Polyn, F. *et al*, *Collect. Czech. Chem. Commun.*, 1968, **33**, 2700 (*hydrate, spec*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley Interscience, 1968, 196 (*rev*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 39, 1978, **C6**, 3 (*rev*)
Sicre, J.E. *et al*, *J. Chem. Soc. A*, 1969, 2878 (*synth, str*)
Schäfer, H. *et al*, *Angew. Chem.*, 1972, **84**, 1130 (*synth, str*)
Sicre, J.E. *et al*, *Inorg. Chem.*, 1972, **11**, 2999, *Rev. J. Chim. Min.*, 1973, **10**, 1 (*str, thermochem*)
Schäfer, H. *et al*, *Angew. Chem. Int. Ed. Engl.*, 1972, **11**, 1030 (*str, thermochem*)
Schäfer, H. *et al*, *Angew. Chem. (Int. Ed. Engl.)*, 1972, **11**, 163 (*rev, thermochem*)
Schäfer, H. *et al*, *Angew. Chem. (Int. Ed. Engl.)*, 1972, **11**, 1030 (*rev, thermochem*)
Schäfer, H. *et al*, *Angew. Chem. (Int. Ed. Engl.)*, 1973, **12**, 300 (*rev, thermochem*)
Sicre, J.E. *et al*, *J. Chem. Soc. A*, 1973, 641, 2782, *Rev. J. Chim. Min.*, 1973, **10**, 1 (*str, thermochem*)
Schäfer, H. *et al*, *Angew. Chem.*, 1973, **85**, 742 (*rev*)
Sicre, J.E. *et al*, *J. Chem. Soc. Dalton*, 1973, 1129 (*str*)
Plies, *Chem. (Engr. Transl.)*, 1973, **47**, 1129 (*str*)
Schäfer, H. *et al*, *Angew. Chem.*, 1973, **85**, 742, *Rev. J. Inorg. Chem. (Engr. Transl.)*, 1973, **12**, 300 (*rev, thermochem*)
Geleznikova, A.I. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 550, *Rev. J. Inorg. Chem. (Engr. Transl.)*, 1983, **28**, 320 (*synth*)

IC-001988

Br_2SeTa

Tantalum(*V*) bromide selenide ($TaBr_2Se$), 1Cl

[50906-76-1]



M 499.6
Probably polymeric as shown based on ir evidence. Synth. from $TaBr_5$ and Sb_2Se_3 in CS_2 at 50° or by heating $TaBr_5$ and Sb_2Se_3 at 140° for 14 days. Brown solid.

Fowles, G.W.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1976, 552 (*synth*)
Nh. Bohn, L. *Suisc Malaya.*, 1981, **10**, 20 (*synth, ir*)

IC-001989

Br_2SeW

Tungsten(*V*) bromide selenide (WBr_2Se)

[58760-83-3]

$WSeBr_2$

M 502.5
Synth. from Sb_2Se_3 and WBr_5 at 120° (v. sensitive to reaction temp.). Red-brown solid. Disproportionates to $WSeBr_4$ and $WSeBr_2$ at 220°.

Brittell, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2191 (*synth*)

IC-001990

Br_3Sm

Samarium(*III*) bromide ($SmBr_3$)

Samarium tribromide

[13759-87-0]

$SmBr_3$

M 390.0
Has $PuBr_3$ struct. Yellow solid. Mp 664°.

Hexahydrate: [13517-12-9].
$Br_3H_{12}O_6Sm$ M 498.1
Deliquescent pale yellow cryst. Sol. H_2O. Loses H_2O >100°. Possesses $NdCl_3.6H_2O$ struct.

Cleve, P.T., *Bull. Soc. Chim. Fr.*, 1885, **43**, 53, 359 (*hydrate, synth*)
Prandtl, W. *et al*, *Z. Anorg. Allg. Chem.*, 1928, **172**, 265 (*synth*)
Klemm, W. *et al*, *Z. Anorg. Allg. Chem.*, 1928, **176**, 181 (*magnetism*)
Selwood, P.W., *J. Am. Chem. Soc.*, 1934, **56**, 2392 (*magnetism*)
Zachariasen, W.H., *Acta Crystallogr.*, 1948, **1**, 265 (*struct*)
Meyer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Haschke, J.M., *Inorg. Chem.*, 1976, **15**, 298 (*hydrate, struct*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 39, 1978, **C6**, 65 (*rev*)
Wood, A.B. *et al*, *Rare Earths Mod. Sci. Technol.*, 1982, **3**, 155 (*synth, str-str*)
Meyer, G. *et al*, *Inorg. Chem.*, 1983, **22**, 3501 (*synth*)
Burns, J.C. *et al*, *Inorg. Chim. Acta*, 1983, **110**, 47 (*lattice, cryst struct*)
Yokoyama, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)
Wilmarth, W.R. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 245 (*raman*)

IC-001991

$Br_3Sn^{\oplus}$

Tribromostannate(*II*)(1−)

[17092-59-6]

$[SnBr_3]^{\oplus}$

M 358.4 (ion)
Cs salt: see *Caesium tin bromide* (Cs_3SnBr_5), IC-001918
NH_4 salt: [37410-16-5].
Cryst. from an aq. soln. of $SnBr_2$ and $[NH_4]Br$. Cryst. + $1H_2O$.

Rimbach, E. *et al*, *Z. Anorg. Allg. Chem.*, 1915, **94**, 139 (*synth*)
Bird, S.R.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1950 (*mössbauer*)
Bird, S.R.A. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 934 (*ir, raman*)
Andersson, I., *Acta Chem. Scand., Ser. A*, 1976, **30**, 229 (*cryst struct*)
Yamada, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 4203 (*npr, mössbauer, struct, synth*)

IC-001992

Br_5Ta

Tantalum bromide ($TaBr_5$), 11Cl

Tantalum tribromide

[13842-73-4]

$TaBr_5$

M 420.6
Synth. from $TaBr_5$ and Ta in a temp. gradient. Grey-green solid. Disprop. above 220° to $TaBr_5$ + $TaBr_2$, and at higher temps. to $TaBr_5$ + $TaBr_{2.5}$.

Young, R.C. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 1740 (*synth*)
Berdonosov, S.S. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, **7**, 1125 (*synth*)
Schäfer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **420**, 1 (*thermal dec*)

IC-001993

Br_3Tb

Terbium(*III*) bromide ($TbBr_3$)

Terbium tribromide

[14456-47-4]

$TbBr_3$

M 398.6
White solid. Sol. H_2O. Mp 827°. Bp 1490°.

Hexahydrate: [15162-98-8]. *Hexaaquadibromoterbium(1+) bromide*
$Br_3H_{12}O_6Tb$ M 506.7
Colourless cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Formulated as $[TbBr_2(OH_2)_6]^{\oplus}Br^{\ominus}$.

Meyer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*hexahydrate, synth, cryst struct*)
Basile, L.J. *et al*, *J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 39, 1978, **C6**, 73 (*rev*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

Br_5Tl

Titanium bromide ($TiBr_5$), 11Cl IC-001994

Titanium tribromide

[13135-31-4]

$TiBr_5$

M 287.5
Struct. resembles a-$TiCl_3$. Synth. by vapour phase transport from Ti, Br_2 and Al_2Br_6; by reaction of $TiCl_3$ with BBr_3 or by reducing $TiBr_4$ with Al at 250° or with Ti at 550°. Can be used in removal of basic N from lubricating oil. Catalyst component. Grey-black solid. Disproportionates to $TiBr_4$ and $TiBr_2$ above 350°. Mp 39°. Bp 230°. Weakly paramagnetic.

Fowles, G.W.A. *et al*, *J. Chem. Soc. A*, 1968, 198 (*synth*)
Moreland, B.G. *et al*, *J. Less-Common Met.*, 1970, **22**, 369 (*synth, cryst struct*)
Droit, P.M. *et al*, *J. Chem. Soc. A*, 1971, 3595 (*synth*)
Schaefer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **474**, 135 (*synth*)
Canadian Pat., 1 172 195, (1984); *CA*, **101**, 213808k (*use*)

Br_5Tl

Thallium(*III*) bromide ($TlBr_3$) IC-001995

Thallium tribromide

[13701-90-1]

$TlBr_3$

M 444.0
Highly unstable. Synth. by adding Br_2 to suspension of $TlBr_2$ in inert solv. Used in synth. of organothallium compds., in oxidation of org. compds., eg. ethylene → ethylene glycol.

▷ Toxic.

Tetrahydrate: Obt. from the anhydr. compd. in aq. soln. Orthorhombic pale yellow needles. Dec. to $Tl_2Br_6.H_2O$, Br_2 at 30°. Sol. H_2O (yellow soln.). Trigonal bipyramidal at Tl (2 axial O and 3 equatorial Br).

Maher, J.P. *et al*, *J. Chem. Soc.*, 1965, 637 (*synth, reaction*)
Glaser, J., *Acta Chem. Scand., Ser. A*, 1979, **33**, 789 (*struct*)
Brady, F. *et al*, *J. Org. Chem.*, 1979, **165**, 21 (*reaction*)
Harase, I. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1989, 68 (*reaction*)

Br_3Tm

Thulium(*III*) bromide ($TmBr_3$) IC-001996

Thulium tribromide

[14456-51-0]

$TmBr_3$

M 408.6
White solid. Sol. H_2O. Mp 952°. ~ 1440°°.

Hexahydrate: [15163-00-5].
$Br_3H_{12}O_6Tm$ M 516.7
Colourless cryst. Sol. H_2O. Loses H_2O on controlled heating *in vacuo*. Isostructural with corresp. chloride.

Meyer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, tga*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*hexahydrate, synth, cryst struct*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1968, 1889 (*struct, ir*)
Basile, L.J. *et al*, *J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 39, 1978, **C6**, 3, 75 (*rev*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

Br_3U

Uranium(*III*) bromide (UBr_3) IC-001997

Uranium tribromide

[13470-19-4]

UBr_3

M 477.7
Possesses the UCl_3 struct. Synth. from UH_3 + HBr or U/Br_2. Hygroscopic red needles. Sol. H_2O. Mp 730° (?27°). Bp 1537°.

▷ Reportedly attacks glass at high temps.

Katz, J.J. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1960, **2**, 255.
Corbett, J.D. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **25**, 1287 (*synth*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1757 (*synth*)
Bullock, J.I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 684 (*synth*)
Taylor, J.C. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 2803 (*cryst struct*)
Levy, J.H. *et al*, *J. Less-Common Met.*, 1975, **39**, 265.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1217 (*synth*)

$Br_3V^{\oplus}$

Tribromovanadate(*II*)(1−), 11Cl IC-001998

$[VBr_3]^{\oplus}$

M 290.6 (ion)
Salts have $CsNiCl_3$ struct. All salts are weakly antiferromagnetic with Néel temps. in the range 13-23K. Other alkali metal, and $NH_4^{\oplus}$ salts are known. The NaBr/VBr_3 system is purely eutectic, others show compd. formation.

K salt: [66752-78-1].
Br_3KV M 329.7
Synth. like the Cs salt. Brown solid.

Cs salt: [43645-25-6].
Br_3CsV M 423.5
Synth. by melting CsBr and VBr_2 or by electrolytic reduction of V(*V*) in aq. HBr with addn. of CsBr. Brown solid. Paramagnetic: μ_{eff} = 2.39μ_B (298K); 1.64μ_B (100K). *T*, 20.4K.

Cs salt, trihydrate: [38832-64-3].
Synth. by mixing CsBr and VBr_2 in aq. HBr. Green solid. A violet hexahydrate is also known (see Hexaaquavanadium(*II*)(2+), IC-019904).

Tl salt: [66752-76-9]. *Thallium(I) tribromovanadate(II)*
Br_3TlV M 495.0
Synth. by melting TlBr and VBr_2.

[38833-79-5]

Siefert, H.J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 949 (*synth, ir, uv-vis, magnetism*)
Siefert, H.J. *et al*, *J. Therm. Anal.*, 1978, **13**, 33 (*phase diagram, synth*)
Hauser, A. *et al*, *J. Solid State Chem.*, 1985, **56**, 343 (*cryst struct, magnetism*)

Br_3V

Vanadium bromide (VBr_3), 11Cl IC-001999

Vanadium tribromide

[13470-26-3]

VBr_3

M 290.6

Hcp with V in octahedral sites (BiI_3 struct.). Synth. from V + Br_2 at 550° in a flow-system or from VCl_3 + BBr_3. Black solid, violet vapour. Disprop. to VBr_4 + VBr_2, thermal dec. to VBr_2 + Br_2. Sol. donor solvs. ΔH_f° −447 kJ mol^{-1}. Paramagnetic, μ_{eff} = 2.67μ_B (293K), 2.51μ_B (90K).

▷ Toxic. YW2750000.

Klemm, W. *et al*, *Z. Anorg. Allg. Chem.*, 1936, **226**, 359 (*magnetism*)
Shchukarev, S.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 345 (*thermochem*)
McCarley, R.E. *et al*, *Inorg. Chem.*, 1964, **3**, 50 (*synth, cryst struct*)
Druce, P.M. *et al*, *J. Chem. Soc. A*, 1971, 3595 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1413 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3457 (*haz*)

IC-002000

Br_3Y

Yttrium(*III*) bromide (YBr_3)

Yttrium tribromide

[13469-98-2]

YBr_3

M 328.6

Can be synth. from YH_2 or YH_3 and Br_2 at 450°; or by heating $(NH_4)_3YBr_6$ *in vacuo* at 350-400°. Deliquescent white cryst. Sol. H_2O, EtOH. Mp 904° (912°).

Hexahydrate: [15163-02-7].

$Br_3H_{12}O_6Y$ M 436.7

Deliquescent colourless cryst. V. sol. H_2O. Loses H_2O on controlled heating *in vacuo* at 60-170°/0.002 mm. Prob. isostructural with corresp. chloride.

Mayer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, ips*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*hexahydrate, synth, struct*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1968, 1889 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, C6, 53 (*rev*)
Sengodan, V. *et al*, *Indian J. Phys., B*, 1979, **53**, 288 (*ir*)
Golovanova, A.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 330 (*synth*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

IC-002001

Br_3Yb

Ytterbium(*III*) bromide ($YbBr_3$)

Ytterbium tribromide

[13759-89-2]

$YbBr_3$

M 412.7

Can be synth. from YbH_2 + Br_2 at 450-500° or by heating $(NH_4)_3YbBr_6$ *in vacuo* at 350°. Colourless cryst. Sol. H_2O. Mp 956° (940°) dec.

Hexahydrate: [15163-03-8].

$Br_3H_{12}O_6Yb$ M 520.8

Colourless cryst. Sol. H_2O. Isostructural with corresp. chloride. Loses H_2O on controlled heating *in vacuo*.

[13813-44-0]

Mayer, I. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1905 (*hexahydrate, synth, ips*)
Brown, D., *Halides of the Lanthanides and Actinides*, Wiley-Interscience, 1968, 194 (*rev*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1968, 1889 (*hexahydrate, synth, cryst struct*)
Basile, L.J. *et al*, *J. Chem. Phys.*, 1971, **55**, 3729 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1978, C6, 76 (*rev*)
Golovanova, A.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 330 (*synth*)
Uwamino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2263 (*pe*)
Meyer, G. *et al*, *J. Less-Common Met.*, 1987, **127**, 155 (*synth*)

IC-002002

$Br_3Zn^{\ominus}$

Tribromozincate(1−)

[18252-07-8]

$[ZnBr_3]^{\ominus}$

M 305.1 (ion)

In polar solvs., anion exists as $[ZnBr_3(solv.)]^{\ominus}$: unsolvated salts known in gas phase; many salts in the solid state, apparently containing $[ZnBr_3]^{\ominus}$ have been shown to contain $[Zn_2Br_6]^{2\ominus}$. See also Aquatribromozincate(1−), IC-001934.

Li salt: [23653-52-3].

Br_3LiZn M 312.0

Na salt: [34150-79-3]. *Sodium tribromozincate* (*$NaZnBr_3$*). *Sodium zinc bromide* (*$NaZnBr_3$*)

Br_3NaZn M 328.0

Formed in vapour phase from NaBr and $ZnBr_2$ at 495-550°.

Lengyel, T., *Acta Chim. (Budapest)*, 1970, **64**, 331; *CA*, **73**, 134397 (*form const of ion*)
Gregory, N.W. *et al*, *J. Phys. Chem.*, 1971, **75**, 3028 (*vapour phase, Na salt formn*)
Waters, D.N. *et al*, *J. Mol. Struct.*, 1973, **17**, 389 (*ir, raman in soln*)
Gorenbein, E.Ya. *et al*, *Zh. Obshch. Khim.*, 1974, **44**, 2391; *Ukr. Khim. Zh. (Russ. Ed.)*, 1974, **40**, 923 (*stab const, Li salt*)

IC-002003

Br_3Zr

Zirconium bromide ($ZrBr_3$), 11Cl

Zirconium tribromide

[24621-18-9]

$ZrBr_3$

M 330.9

Struct. comprises chains of face-sharing octahedra with equally spaced Zr atoms. Non-stoichiometric in the range 2.8 ⩽ Zr:Br ⩽ 3.32 (435°), 2.83 (775°) with lattice constants decreasing smoothly as Br content increases. Synth. by reducing $ZrBr_4$ with Zr or Al. Absorbent in artificial kidneys (see also Zirconium bromide ($ZrBr_2$), IC-001901 and Zirconium bromide ($ZrBr_4$), IC-002090). Blue-black solid if synth. above 485° otherwise a dark green polymorph is formed. Both disproportionate at 500° → $ZrCl_2$ and $ZrCl_4$.

Canterford, J.H. *et al*, *Halides of the Second and Third Row Transition Metals*, Wiley, New York, 1968 (*rev*)
Larsen, E.M. *et al*, *Inorg. Chem.*, 1974, **13**, 574 (*synth*)
Kleppinger, J. *et al*, *Inorg. Chem.*, 1975, **14**, 3128 (*synth, cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1354 (*synth*)
Daake, R.L. *et al*, *Inorg. Chem.*, 1978, **17**, 1192 (*synth, stoichiometry*)
Corbett, J.D. *et al*, *Proc. Electrochem. Soc.*, 1978, 78 (*synth*)
Larsen, E.M. *et al*, *Inorg. Chem.*, 1982, **21**, 2619 (*cryst struct*)
Japan. Pat., 60 132 644, (1985); *CA*, **104**, 56466g (*use*)

$Br_4Cd^{2\ominus}$

Tetrabromocadmate(2−) IC-002004

[15844-14-1]

$[CdBr_4]^{2\ominus}$

M 432.0 (ion)

Di-Cs salt: [16593-59-2].

Br_4CdCs_2 M 697.8

Phase in the CsBr-$CdBr_2$ system. Cryst. with β-K_2SO_4 struct. Undergoes phase transitions at 252, 237 and 158K. Mp 457°.

Bis-Et_4N salt: [29890-60-6].

White cryst. (aq. EtOH). Mp 297°.

Il'yasov, I.I., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 766 (*synth, Cs salt*)
Davies, J.E.D. *et al*, *J. Chem. Soc. A*, 1968, 2054 (*ir, raman*)
Ross, S.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1611 (*synth*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1914 (*synth, ir, raman*)
Ackerman, J.J.H. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 341 (*synth, Cd-113 nmr*)
Altermatt, D. *et al*, *Acta Crystallogr., Sect. B*, 1984, **40**, 357 (*cryst struct, Cs salt*)

$Br_4ClCu^{3\ominus}$

Tetrabromochlorocuprate(*II*)(3−), 10Cl IC-002005

$[CuClBr_4]^{3\ominus}$

M 418.6 (ion)

Square pyramidal geometry at Cu. Corresp. pentabromo compd. non-existent.

N-(2-Ammoniumethyl)piperazinium salt: [73233-33-7].

Brown solid + H_2O. Mp 187° dec. μ_{eff} = 1.79μ_B.

Antolini, L. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 1303 (*synth, ir, ue, magnetism*)

$Br_4ClH_2OPt^{\ominus}$

Aquatetrabromochloroplatinate(*IV*)(1−), 9Cl IC-002006

$[(H_2O)PtBr_4Cl]^{\ominus}$

M 568.1 (ion)

Not isol. Prep. *in situ* for kinetic substitution studies by Cl_2 + $[PtBr_4]^{2\ominus}$ in H_2O. Isomerism not investigated.

Elding, L.I. *et al*, *Inorg. Chim. Acta*, 1977, **24**, 239 (*synth*)

$Br_4Cl_8W_6$

Tetrabromooctachlorohexatungsten IC-002007

Tungsten bromide chloride (*$W_6Br_4Cl_8$*)

[12049-05-7]

$(W_6Cl_8)Br_4$

M 1706.3

Prepd. from $(W_6Cl_8)Cl_4$ by halide exchange with HBr. Cryst.

[107739-55-9, 107739-56-0]

Mattes, R. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **357**, 30 (*ir*)
Hogue, R.D. *et al*, *Inorg. Chem.*, 1970, **9**, 1354 (*synth, ir*)

$Br_4Cr^{3\ominus}$

Tetrabromochromate(*II*)(2−), 11Cl, 10Cl, 9Cl IC-002008

$[CrBr_4]_n^{2n\ominus}$ sheets

M 371.6 (ion)

Salts are ferromagnetic. Struct. and props. prob. as Tetrachlorochromate(*II*)(2−), IC-016988.

Di-Cs salt: [51159-52-5]. *Caesium tetrabromochromate* (*Cs_2CrBr_4*)

Br_4CrCs_2 M 637.4

Air-sensitive dark green powder. Ferromagnetic.

Di-NH_4 salt: [51181-52-3].

Air-sensitive orange-brown powder. Antiferromagnetic; struct. unknown.

Bis-$MeNH_3$ salt: [77135-52-5].

Air-sensitive greenish-yellow cryst. Ferromagnetic, other monoalkylammonium salts also known.

Bis-Me_2NH_2 salt: [77135-51-4].

Light-green air-sensitive cryst. Antiferromagnetic; struct. unknown.

Bis-pyridinium salt: [51159-54-7].

Air-sensitive yellow solid. Antiferromagnetic; struct. unknown.

Bis-$PhCH_2NH_3$ salt: [102629-61-8].

Yellow air-sensitive cryst. Ferromagnetic.

[63949-49-5]

Babar, M.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 27 (*synth, magnetism, ue, ir*)
Bellitto, C., *J. Magn. Magn. Mater.*, 1986, **54-57**, 1495 (*synth, magnetism*)

Br_4Cr

Chromium(*IV*) bromide ($CrBr_4$) IC-002009

Chromium tetrabromide. Tetrabromochromium(IV)

[23098-84-2]

$CrBr_4$

M 371.6

Tetrahedral struct. proposed. Synth. from $CrBr_3$ and excess Br_2 at high temp. Gas at high temp.

Ciuni, B. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 247 (*synth, raman*)

$Br_4CrH_4O_2^{1\ominus}$

Diaquatetrabromochromate(*II*)(2−), 11Cl, 10Cl, 9Cl IC-002010

$[CrBr_4(OH_2)_2]^{\ominus}$

M 407.6 (ion)

Distorted octahedral anion; see also Diaquadibromochromium(*II*), IC-001783. Salts crystallise from halides in HBr aq. Salts are high spin; thermal dehydration gives salts of Tetrabromochromate(*II*)(2−), IC-002008.

Di-Rb salt: [50774-41-9]. *Rubidium diaquatetrabromochromate*(II). *Rubidium tetrabromochromate*(II) *dihydrate*

$Br_4CrH_4O_2Rb_2$ M 578.5

Light blue air-sensitive cryst. (HBr).

Di-Cs salt: [50937-51-4]. *Caesium diaquatetrabromochromate*(II). *Caesium tetrabromochromate*(II) *dihydrate*

$Br_4CrCs_2H_4O_2$ M 673.4

Light blue air-sensitive cryst. (HBr).

Di-NH_4 salt: [77209-50-8].

Light turquoise air-sensitive cryst. (HBr).

Bis-pyridinium salt: see Diaquadibromochromium(II), IC-001783

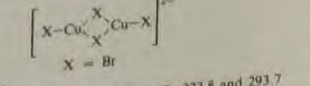
[50774-42-0]

Babar, M.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 27 (*synth, props*)
Ladd, M.F.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 2351

$Br_4Cu_2^{2\ominus}$ IC-002011

Di-μ-bromodibromodicuprate(*I*)(2−)

Dibromocuprate(I−) dimer



X = Br

M 446.7 (ion)
Discrete centrosymmetric dimer. Cu—Cu 273.8 and 293.7 pm.
Bis-Et_4N salt: [91514-35-1]
Colourless fibrous cryst. (ethyl formate).
Bis-benzyltrimethylammonium salt: [98912-85-7].
Colourless prisms (EtOH).

Bowmaker, G.A. *et al, Aust. J. Chem.*, 1973, **26**, 79 (*synth*)
Asplund, M. *et al, Acta Chem. Scand., Ser. A*, 1984, **38**, 135 (*synth, cryst struct, Et_4N salt*)
Andersson, S. *et al, Acta Chem. Scand., Ser. A*, 1985, **39**, 423 (*synth, cryst struct, benzyltrimethylammonium salt*)

IC-002012

Br_4F_2Mo

Molybdenum bromide fluoride ($MoBr_4F_2$), 9CI

Molybdenum tetrabromide difluoride

$MoBr_4F_2$

M 453.5
The ir spectrum suggests both *cis*- and *trans*-isomers present. Formed in low yield (<1%) in the reaction of $Mo(CO)_6$, Br_2 and MoF_6. Dark red, volatile material.

[25029-60-1, 25029-61-2]

Mercer, M. *et al, J. Chem. Soc. A*, 1969, 2532 (*synth*)

IC-002013

$Br_4Fe^{2\ominus}$

Tetrabromoferrate(*II*)(2−), 11Cl

[33914-62-4]

$[FeBr_4]^{2\ominus}$ (T_d)

M 375.4 (ion)
Characterised by ir absorp. ≃ 220 cm^{-1}.
Bis-Et_4N salt: Synth. from $FeBr_2.2H_2O$ + $[Et_4N]Br$ in EtOH. Cream-coloured needles (stable to oxidn when dry) or pale brown cryst. (EtOH).

Gill, N.S., *J. Chem. Soc.*, 1961, 3512 (*synth, uv, magnetism*)
Inorg. Synth., 1967, **9**, 138 (*synth*)
Colton, R. *et al, Halides of the First Row Transition Metals*, Wiley, NY, 1969, 306 (*rev, bibl*)
Pelikan, P. *et al, Collect. Czech. Chem. Commun.*, 1984, **49**, 2837 (*bonding*)

IC-002014

$Br_4Fe^{\ominus}$

Tetrabromoferrate(*III*)(1−), 11Cl

[20519-31-7]

$[FeBr_4]^{\ominus}$ (T_d)

M 375.4 (ion)
Catalyst. Useful large anion for precipitation of salts. Has been used in extraction of Fe. Readily hydrol.
Cs salt: [83779-08-2]. *Caesium iron(III) bromide ($CsFeBr_4$)*
Br_4CsFe M 508.3
Ph_4P salt: Golden-brown leaflets. Mp 105-106°. On melting, evolves HBr.
Et_4N salt: [21279-19-6].
Synth. from $FeBr_3$ + $[Et_4N]Br$. Cryst. (hot EtOH). Sol. Me_2CO. μ_{eff} = 1.52 (1.4K), 6.02μ_B (298K).

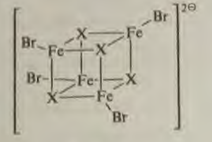
Sheldon, J.C. *et al, J. Am. Chem. Soc.*, 1958, **80**, 2117 (*synth, Ph_3PH salt*)
Ginsberg, A.P. *et al, Inorg. Chem.*, 1963, **2**, 817 (*synth, magnetism, Et_4N salt*)
Clausen, C.A. *et al, Inorg. Chem.*, 1970, **9**, 220 (*ir, mössbauer, synth*)
Rodriguez, F. *et al, Transition Met. Chem.*, 1985, **10**, 351 (*esr*)
Muraoka, T. *et al, Inorg. Chim. Acta*, 1986, **124**, 49 (*mcd*)

$Br_4Fe_4S_4^{2\ominus}$ IC-002015

Tetrabromotetra-μ_3-thioxotetraferrate(2−), 11Cl

Tetrabromotetra-μ_3-sulfidotetraferrate(2−)

[65107-38-2]



X = S

M 671.2 (ion)
Mixed oxidation state 2Fe(*III*)2Fe(*II*) compd. Synthetic model for ferredoxins. Precursor to higher nuclearity clusters.
Bis-Et_4N salt: [65208-04-0].
Obt. by reaction of $FeBr_3$ + NaSPh + $[Et_4N]Br$ in MeCN with S. Black cryst. Insol. Et_2O; sol. MeCN. Iodo analogue similarly prepd.
Bis-Ph_4P salt: [97225-95-1].
Obt. by bubbling H_2S through $FeSO_4.7H_2O$ in DMF containing $[Ph_4P]Br$ in presence of O_2.

Wong, G.B. *et al, Inorg. Chem.*, 1978, **17**, 578 (*synth, magnetism, spectra, electrochem*)
Mueller, A. *et al, Chimia*, 1985, **39**, 23, 24 (*synth, cryst struct*)
Mueller, A. *et al, Naturwissenschaften*, 1986, **73**, 669 (*synth*)
Rutchik, S. *et al, Inorg. Chem.*, 1988, **27**, 1513 (*synth, cryst struct*)
Coucouvanis, D. *et al, Inorg. Chem.*, 1988, **27**, 4066 (*synth*)

$Br_4Fe_4Se_4^{2\ominus}$ IC-002016

Tetrabromotetra-μ_3-selenotetraferrate(2−)

As Tetrabromotetra-μ_3-thioxotetraferrate(2−), IC-002015 with

X = Se

M 858.8 (ion)
Bis-Et_4N salt: [113748-21-3].
Synth. from $FeBr_3$, Na_2Se, $[Et_4N]Br$ in DMF. Black cryst. μ_{eff} = 2.19μ_B (302K).

Rutchik, S. *et al, Inorg. Chem.*, 1988, **27**, 1513 (*struct, synth*)

$Br_4Ga^{\ominus}$ IC-002017

Tetrabromogallate(*III*)(1−)

[17611-23-3]

$[GaBr_4]^{\ominus}$

M 389.3 (ion)
λ 103.1 Ω^{-1} cm^2 mol^{-1}.
Na salt: [30487-88-8].
Br_4GaNa M 412.3
Synth. from NaBr + $GaBr_3$. Colourless moisture sensitive cryst. (melt). Mp 190°.
K salt: [50328-30-8].

Br_4GaK M 428.4
Synth. from KBr + $GaBr_3$. Colourless moisture-sensitive cryst. (melt). Mp 196°.
Rb salt: [52582-08-8].
Synth. from RbBr + $GaBr_3$. Colourless moisture-sensitive cryst. (melt). Mp 252°.
Cs salt: [52582-09-9].
Synth. from CsBr + $GaBr_3$. Colourless moisture-sensitive cryst. (melt). Mp 320°.
Et_4N salt: [33896-84-3].
$C_8H_{20}Br_4GaN$ M 519.5
Electrochemical synth. from Ga, Br_2 and $[Et_4N]Br$ in MeOH-C_6H_6 (1:4). Yellow cryst. Spar. sol. C_6H_6, MeOH, Et_2O.
Tetrabutylammonium salt: [34249-07-5].
Electrochemical synth. Cream-coloured cryst. ($CHCl_3/Et_2O$). Sol. $CHCl_3$; spar. sol. Et_2O.
Tl salt: [52582-10-2].
Br_4GaTl M 593.7
Colourless moisture-sensitive cryst. Mp 184°.

Akitt, J.W. *et al, J. Chem. Soc.*, 1965, 4410 (*Ga-71 nmr*)
Dudareva, A.G. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 1174; 1974, **19**, 874 (*phase diagram*)
Schmulbach, C.D., *Inorg. Chem.*, 1971, **10**, 1902 (*cond*)
Work, R.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 1537 (*ir*)
Mascherpa Corral, D. *et al, Bull. Soc. Chim. Fr.*, 1973, 1912 (*phase diagram*)
Buslaev, Yu.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1974, **216**, 796 (*Ga-71 nmr*)
Andrews, S.P. *et al, J. Chem. Res. (S)*, 1978, 94 (*ir, raman*)
Molodkin, A.K. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1980, **25**, 1244 (*phase diagram*)
Fichter, W. *et al, Z. Naturforsch., B*, 1980, **35**, 170 (*nqr*)
Colton, R. *et al, Aust. J. Chem.*, 1981, **34**, 949 (*Ga-71 nmr*)
Inorg. Synth., 1983, **22**, 135 (*synth*)
Taylor, M.J. *et al, Polyhedron*, 1990, **9**, 207 (*Ga-71 nmr*)

Br_4GaIn IC-002018

Gallium indium bromide ($GaInBr_4$)

$Br_2Ga—InBr_2$

M 504.1
Isol. as complexes. Synth. from fused Ga, $GaBr_3$, In, $InBr_3$ mixture.
Bis-THF complex: [81182-68-5].
Dibromo[dibromo(tetrahydrofuran)gallium](tetrahydrofuran)indium, 10CI
$C_8H_{16}Br_4GaInO_2$ M 648.3
White solid.
Bis-tetrahydropyran complex: [81182-66-3].
Dibromo[dibromo(tetrahydro-2H-pyran)gallium](tetrahydro-2H-pyran)indium, 10CI
$C_{10}H_{20}Br_4GaInO_2$ M 676.4
White solid.
Bis-dioxan complex: [81182-64-1]. *Dibromo[dibromo(1,4-dioxane-O^1)gallium](1,4-dioxane-O^1)indium, 10CI*
$C_8H_{16}Br_4GaInO_4$ M 680.3
White solid.
Piperazine complex: [81182-60-7].
White solid.

Sinclair, I. *et al, Inorg. Nucl. Chem. Lett.*, 1981, **17**, 279 (*synth, complexes*)

Br_4Ga_2 IC-002019

Gallium(*I*) tetrabromogallate(*III*)

[18897-61-5]

$Ga[GaBr_4]$

M 459.0
Formerly described as Gallium(*II*) bromide. From Ga + $GaBr_3$ at 180°. White moisture-sensitive solid. Mp 167°. Many complexes descr. See e.g. Tetrabromobis(1,4-dioxane-O^1)digallium, IC-006067.
Tetrabromobis(pyridine)digallium, IC-006782.
Conductivity 15.5 Ω^{-1} m^{-1} at 170°.
'Monomer':
Br_3Ga M 229.5

Woodward, L.A. *et al, J. Chem. Soc.*, 1958, 1505 (*synth, raman*)
Greenwood, N.N. *et al, J. Chem. Soc.*, 1958, 1680 (*props*)
Ali, S.M. *et al, J. Inorg. Nucl. Chem.*, 1959, **9**, 124 (*complexes*)
Inorg. Synth., 1960, **6**, 33 (*synth*)
Beamish, J.C. *et al, Inorg. Chem.*, 1978, **17**, 2026 (*synth*)
Okuda, T. *et al, Bull. Chem. Soc. Jpn.*, 1985, **58**, 2731.

Br_4Ge IC-002020

Germanium bromide ($GeBr_4$)

Germanium tetrabromide. Tetrabromogermane

[13450-92-5]

$GeBr_4$

M 392.2
Grey-white octahedral cryst. Dec. in H_2O; sol. EtOH, Et_2O, C_6H_6. d^{30} 2.1. Mp 26°. Bp 186°.
▷ LY5220000.

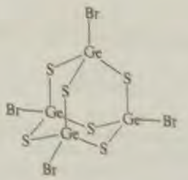
Andrews, S.P. *et al, J. Chem. Res. (S)*, 1978, 94 (*ir, raman*)
Buerger, H. *et al, J. Mol. Spectrosc.*, 1983, **97**, 266 (*ir*)
van der Kerk, S.M., *Polyhedron*, 1983, **2**, 509 (*rev*)
Buerger, H. *et al, Z. Naturforsch., A*, 1984, **39**, 871 (*ir*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1801.

$Br_4Ge_4S_6$ IC-002021

Germanium bromide sulfide ($Ge_4Br_4S_6$)

1,3,5,7-Tetrabromo-2,4,6,8,9,10-hexathia-1,3,5,7-tetragermatricyclo[3.3.1.1^{3,7}]decane, 9CI. Tetragermanium tetrabromide hexasulfide

[58356-00-6]



M 802.4
Adamantane-like struct. Synth. by adding H_2S to a boiling soln. of $GeBr_4$ in CS_2. Cryst. Mp 305° dec.

Pohl, S., *Angew. Chem., Int. Ed. Engl.*, 1976, **15**, 162 (*synth, cryst struct, raman*)
Pohl, S. *et al, Z. Naturforsch., B*, 1981, **36**, 1432 (*cryst struct, raman*)

$Br_4HIOPt^{2\ominus}$ IC-002022

Tetrabromohydroxyiodoplatinate(*IV*)(2−), 9CI

[54374-98-0]

$[Pt(OH)Br_4I]^{2\ominus}$

M 658.6 (ion)

Not isol. One product formed from reaction of $I^{\ominus}$ with $[PtBr_4]^{2\ominus}$ in H_2O at high pH. Isomerism not investigated.

Johnson, D.W. et al, Can. J. Chem., 1974, 52, 3083.

IC-002023

Br_4HSb

Hydrogen tetrabromoantimonate(*III*)(1−), 8CI

Tetrabromoantimonic(III) acid

$H[SbBr_4]$

M 442.3

Salts synth. from $SbBr_3$ + amine in HBr aq.

Et_2NH salt: [59450-14-5].
Solid. Mp 120-126°.

Et_3N salt: [38333-03-8].
Solid. Mp 192°.

Aniline salt: [54205-54-8].
Solid. Mp 128°.

Py salt: [52279-30-8]
$C_5H_6Br_4NSb$ M 521.4
Pale yellow needles or yellow plates (MeCN). Mp 126° (216-217.5°). Octahedrally coordinated anion. Interatomic distance: Sb—Br 256.4-282.2 pm.

Quinoline salt: [52279-33-1].
Light yellow needles. Mp 245°.

Isoquinoline salt: [52279-34-2].
Mp 260-263°.

Gmelin Handbook Inorg. Chem., Syst. No. 18, 1949, 482 (rev, bibl)
Jha, N.K. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 2953; 1974, **36**, 1479; 1976, **38**, 401 (*synth*)
Hooper, H.A. *et al, Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)
Stewart, J.M. *et al, Inorg. Chem.*, 1974, **13**, 2767 (*synth, cryst struct*)
Dettaven, P.W. *et al, Cryst. Struct. Commun.*, 1976, **5**, 31 (*cryst struct*)
Hedgen, S.W. *et al, Inorg. Chem.*, 1984, **23**, 1458 (*synth, raman, mössbauer*)
Okuda, T. *et al, Z. Naturforsch., A*, 1986, **41**, 319 (*spr*)
Okuda, T. *et al, J. Chem. Soc., Dalton Trans.*, 1989, 631 (*spr*)

IC-002024

$Br_4H_2IOPt^{\ominus}$

Aquatetrabromoiodoplatinate(*IV*)(1−), 9CI

[54374-97-9]

$[(H_2O)PtBr_4I]^{\ominus}$

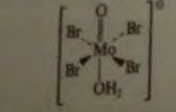
M 659.6 (ion)
Not isol. One product from reaction of $I^{\ominus}$ with $[PtBr_4]^{2\ominus}$ in H_2O. Isomerism not investigated.

Johnson, D.W. et al, Can. J. Chem., 1974, 52, 3083 (synth)

IC-002025

$Br_4H_2MoO_3^{\ominus}$

Aquatetrabromooxomolybdate(*V*)(1−), 10CI, 9CI



M 449.5 (ion)
trans-Octahedral anion, interatomic distances (av.): Mo=O 162, Mo—Br 253, Mo—OH_2 232 pm. Isomorphous with $[MoOCl_4(OH_2)]^{\ominus}$.

Et_4N salt: [52729-41-6].
Synth. from $[Et_4N]Cl$ and $Mo_2(OAc)_4$ in HBr. Yellow cryst.

Ph_4As salt: [35772-28-2].
Brown tetragonal prisms.

Pyridinium salt: [71096-99-6].
Air-stable yellow cryst. + HBr (HBr). Formulated as $(PyH)_4[MoOBr_4(OH_2)]_2Br_2$.

Seane, J.G., *Acta Crystallogr., Sect. B*, 1967, **23**, 85 (*cryst struct*)
Edwards, A.J. *et al, J. Chem. Soc. A*, 1968, 2503.
Kergoat, R. *et al, Z. Anorg. Allg. Chem.*, 1975, **416**, 174.
Garner, C.D. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1202.
Bino, A. *et al, Inorg. Chem.*, 1979, **18**, 2710 (*cryst struct, synth*)

IC-002026

$Br_4H_2NOOs^{\ominus}$

Aquatetrabromonitridoosmate(*VI*)(1−)

[59187-89-2]

$[N{\equiv}OsBr_4(OH_2)]^{\ominus}$ (C_{4v})

M 541.8 (ion)

K salt: [62121-43-1].
Orthorhombic cryst. + $1H_2O$.

Tetrapropylammonium salt: [59187-90-5].
Synth. from $[Pr_4N]Cl$ and $K[OsO_3N]$ in HBr.

Cleare, M.J. *et al, J. Chem. Soc. A*, 1970, 1117 (*use*)
Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*use*)
Cowman, C.D. *et al, Inorg. Chem.*, 1976, **15**, 1747 (*use*)
Tkachev, V.V. *et al, Zh. Strukt. Khim.*, 1976, **17**, 940 (*cryst struct*)
Sen, D. *et al, Indian J. Chem.*, 1978, **1617**, 859 (*props*)
Wright, M.J. *et al, Transition Met. Chem.*, 1982, **7**, 53 (*use*)
Nefedov, V.I. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1986, **291**, 614 (*pe*)
Kravchenko, E.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1987, **294**, 130 (*spr*)

IC-002027

$Br_4H_2O_2Re^{\ominus}$

Aquatetrabromooxorhenate(*V*)(1−)

$[O{=}ReBr_4(H_2O)]^{\ominus}$

M 539.8 (ion)
Aqua complex of Tetrabromorhenate(*V*)(1−). IC-002051. Octahedral.

trans-form
Interatomic distances: Re=O ~ 171, Re—OH_2 ~ 232, Re—Br ~ 251 pm.

Et_4N salt: [35788-72-8].
Synth. from $ReBr_3$ and Et_4NBr in 48% HBr in air. Ruby-red cryst.

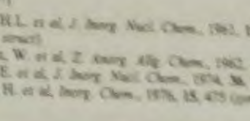
Cotton, F.A. *et al, Inorg. Chem.*, 1965, **4**, 1627; 1966, **5**, 9 (*synth, cryst struct, ir, uv, props*)
Shusterovich, E.M. *et al, Zh. Strukt. Khim.*, 1972, **13**, 111 (*struct*)

IC-002028

$Br_4H_2O_2Tc^{\ominus}$

Tetrabromoaquaoxotechnetate(*V*)(1−)

[128642-51-3]



M 452.5 (ion)
trans-Octahedral anion. Prep. by HBr reduction of $TcO_4^{\ominus}$ at −5°.

Et_4N salt: [128642-52-4].
Dichroic green-orange solid. Sol. MeCN, $CHCl_3$, EtOAc. Insol. Et_2O, hydrocarbons. Dec. in alcohols.

Mantegazzi, D. *et al, Inorg. Chim. Acta*, 1989, **167**, 195 (*synth, uv, ir, cryst struct*)

$Br_4H_4InO_2^{\ominus}$

Diaquatetrabromoindate(*III*)(1−) **IC-002029**

$[InBr_4(OH_2)_2]^{\ominus}$

M 470.4 (ion)
trans-Octahedral anion.

K salt: [73515-96-5].
$Br_4H_4InKO_2$ M 509.5
Obt. by slow evaporation of an aq. soln. of $InBr_3$ and KCl. Hygroscopic white cryst. (H_2O).

Wignacourt, J.-P. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 669 (*synth, cryst struct*)

$Br_4H_4O_2Pt$

Diaquatetrabromoplatinum(*IV*), 9CI **IC-002030**

Platinum(IV) *bromide dihydrate. Platinum tetrabromide dihydrate*

[35902-35-3]

$(H_2O)_2PtBr_4$

M 550.7
Not isol. but both isomers formed in aq. solns. containing $Br^{\ominus}$ and $Pt^{2\oplus}$.

[63357-74-4, 63357-75-5]

Elding, L.I. *et al, Inorg. Chim. Acta*, 1971, **5**, 643; 1977, **22**, 201 (*uv, reactions*)

$Br_4H_4O_2Ru^{\ominus}$

Diaquatetrabromoruthenate(*III*)(1−) **IC-002031**

$[Ru(OH_2)_2Br_4]^{\ominus}$

M 456.7 (ion)
Geometry unknown. All the salts are poorly characterised. Sol. H_2O.

Bulvidaite, M., *Z. Anorg. Allg. Chem.*, 1937, **230**, 285 (*synth*)

$Br_4H_4O_2Tc$

Diaquatetrabromotechnetium(*IV*) **IC-002032**

Technetium(IV) *bromide dihydrate*

[113488-89-4]

$TcBr_4(OH_2)_2$

M 454.5
Rare example of H_2O coordinated to technetium (though cf. e.g. (Aqua)pentachlorotechnetate(*IV*)(1−), IC-017173).

Mirch, J.G. *et al, J. Radioanal. Nucl. Chem.*, 1989, **132**, 293.

Br_4Hf

Hafnium bromide ($HfBr_4$), 11CI **IC-002033**

Hafnium tetrabromide

[13777-22-5]

$HfBr_4$

M 498.1
Prob. has SnI_4 struct. in the solid state. Tetrahedral molecule in gas phase. Synth. from HfO_2, Br_2 and C at 400°, by reaction of Hf with molten $PbBr_2$, or $HfCl_4$ with BBr_3, or from Hf and Br_2 at 400°. Colourless to yellow solid. Mp 425°. Subl. 420° in vacuo. ΔH_f° −840 kJ mol^{-1}.

Berdonosov, S.S. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1963, **8**, 277 (*synth, cryst struct*)
Druce, P.M. *et al, J. Chem. Soc. A*, 1971, 3595 (*synth*)
Thomas, W. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 2227 (*synth*)

$Br_4I_6Mo_6$

Octaiodohexamolybdenum tetrabromide **IC-002034**

Molybdenum bromide iodide ($Mo_6Br_4I_6$)

$Mo_6I_6Br_4$

M 1910.4
Presumed to contain clusters of Mo_6 octahedra. Prepd. by addition of HBr to alk. MoI_2 solns.

Sheldon, J.C., *J. Chem. Soc.*, 1962, 410 (*remark*)

$Br_4In^{\ominus}$

Tetrabromoindate(1−) **IC-002035**

[17611-24-4]

$[InBr_4]^{\ominus}$ (T_d)

M 434.4 (ion)
$[InBr_3X]^{\ominus}$ and $[InBr_2X_2]^{\ominus}$ where X = Cl or I are also known.

Me_4N salt: [21288-93-7].
Synth. from aq. $InBr_3$ and $[Me_4N]Br$. Colourless cryst. (4*M* HBr). Mp 236-238°. Other R_4N salts also descr.

Butyltriphenylphosphonium salt: [33751-02-9].
Synth. from aq. $InBr_3$ and $[BuPh_3P]Br$. Colourless cryst. (EtOH). Mp 71°.

Ekeley, J.B. *et al, J. Am. Chem. Soc.*, 1936, **58**, 907 (*synth*)
Woodward, L.A. *et al, J. Chem. Soc.*, 1955, 1599 (*raman*)
Fratiello, A. *et al, Inorg. Chem.*, 1971, **10**, 1627 (*In-115 nmr*)
Gislason, J. *et al, Inorg. Chem.*, 1971, **10**, 1908 (*synth, ir, raman*)
Contreras, J.G. *et al, Inorg. Chem.*, 1972, **11**, 2987 (*calor raman*)
Freeland, B.H. *et al, Can. J. Chem.*, 1977, **55**, 1527 (*mcra*)
Drake, J.E. *et al, Inorg. Chem.*, 1980, **19**, 34 (*related ions*)
McGarvey, B.R. *et al, Inorg. Chem.*, 1980, **19**, 3432 (*In-115 nmr*)
Colton, R. *et al, Aust. J. Chem.*, 1981, **34**, 949 (*In-115 nmr*)

Br_4In_3

Indium(*I*) tetrabromoindate(*III*) **IC-002036**

[33939-40-1]

$In[InBr_4]$

M 549.2
Formerly descr. as $InBr_2$. Synth. from $InBr_3$ and In in hot xylene. Colourless moisture sensitive needles (xylene). Mp 200°.

'Monomer': Indium dibromide (incorr.)
Br_2In M 274.6
Not isol.

[14226-34-7]

Walter, P.H.L. *et al, J. Inorg. Nucl. Chem.*, 1961, **19**, 223 (*synth, powder struct*)
Morawietz, W. *et al, Z. Anorg. Allg. Chem.*, 1962, **316**, 220 (*synth*)
Davies, J.E. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 805 (*raman*)
Freeland, H. *et al, Inorg. Chem.*, 1976, **15**, 475 (*synth, raman*)

$Br_4Mn^{2\ominus}$

Tetrabromomanganate(*II*)(2−) **IC-002037**

$[MnBr_4]^{2\ominus}$ (T_d)

M 374.5 (ion)

Di-Li salt: [78528-06-0]. *Lithium tetrabromomanganate(II)* (Li_2MnBr_4)
Br_4Li_2Mn M 388.4

Synth. from LiBr, Mn and Br_2 in Et_2O. Reacts with $LiAlH_4$ in Et_2O at −80° to give $Mn(AlH_4)_2$.

Di-Cs salt:
Br_4Cs_2Mn M 640.3
Synth. from CsBr and $MnBr_2$ at 650° *in vacuo*. Greenish-yellow hygroscopic cryst. Mp 518°. Rhombic isotype of Cs_2ZnBr_4 and Cs_2CuBr_4.

Bis-Me_2NH_2 salt: Synth. from $[Me_2NH_2]Br$ and $MnBr_2$ in EtOH. Green-yellow needles. Sol. H_2O, MeOH, EtOH, MeCN.

Bis-Et_4N salt: [2536-14-3].
Synth. from $[Et_4N]Br$ and $MnBr_2$ in H_2O, EtOH or $SOBr_2$. Green-yellow needles. Sol. CH_2Cl_2. Mp 300°. $\mu_{eff} = 5.97\mu_B$.

Monnier, G., *Ann. Chim. (Paris)*, 1957, **2**, 14 (*synth, reactions*)
Gill, N.S. *et al*, *J. Chem. Soc.*, 1959, 3997 (*magnetism*)
Cotton, F.A. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 167 (*props, uv*)
Sabatini, A. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 17 (*ir, raman*)
Inorg. Synth., 1967, **9**, 136 (*synth*)
Foster, J.J. *et al*, *J. Chem. Soc. A*, 1968, 2625 (*synth, uv*)
Edwards, H.G.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 540 (*raman*)
Goodyear, J. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 1231 (*synth, cryst struct*)
Seifert, H.-J. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **391**, 302 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, **C5**, 290; 1983, **C10**, 49 (*rev, bibl, uv-vis*)

IC-002038

Br_4Mo

Molybdenum(*IV*) bromide ($MoBr_4$)
Molybdenum tetrabromide
[13520-59-7]

$MoBr_4$

M 415.5
Isomorphous with $MoCl_4$, containing $MoBr_6$ octahedra. Synth. by the bromination of $MoBr_3$ or $Mo(CO)_6$. Additive for special radiation-resistant lubricants. Black needles. V. sol. H_2O. Easily oxidised and hydrolysed. Disproportionates on heating to $MoBr_3$ and Br_2.

Inorg. Synth., 1967, **10**, 49 (*synth*)
Druce, P.M. *et al*, *J. Chem. Soc. A*, 1971, 3595 (*synth*)
Oppermann, H., *Z. Anorg. Allg. Chem.*, 1973, **395**, 249 (*thermodyn*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1537 (*synth*)
Pascal, P., *Nouveau Traité de Chimie Minérale*, 1976, **5**, 61 (*rev*)

IC-002039

$Br_4MoN^{\ominus}$

Tetrabromonitridomolybdate(*VI*)(1−), 10Cl
Tetrabromonitridomolybdate(VI)(*1−*)

$[N{\equiv}MoBr_4]^{\ominus}$

M 429.5 (ion)
Square pyramidal with apical N, Mo—N 163 pm, compatible with triple bond, BrMoN angle 103°. Synth. from $MoNBr_3$ + PPh_4Br in CH_2Br_2 soln.

Ph_4P salt: [76565-24-7].
Hygroscopic brown cryst.

Dehnicke, K. *et al*, *Z. Kristallogr.*, 1980, **153**, 181 (*cryst struct, synth, ir*)

IC-002040

Br_4MoO

Molybdenum(*VI*) bromide oxide ($MoBr_4O$), 9Cl
Molybdenum(VI) *oxytetrabromide*
[21846-56-0]

$MoOBr_4$

M 431.5
Generated using a fused mixt. of an alkali metal bromide with MoO_3 at >250°. Dark brown sublimate.

Ward, B.G. *et al*, *Inorg. Chem.*, 1968, **7**, 2569 (*synth, ir*)

IC-002041

$Br_4NOTc^{\ominus}$

Tetrabromonitrosyltechnetate(1−)

$[TcBr_4(NO)]^{\ominus}$

M 448.5 (ion)
Square pyramidal with axial NO. Formally and operationally Tc(*II*); esr consistent with low-spin d^5 config. Synth. from reaction of $TcO_2{\cdot}xH_2O$ with NO in 4*M* HBr. Starting material for prep. of complexes with $TcNO^{3\oplus}$ core; reacts with $NCS^{\ominus}$ to give $[Tc(NO)(NCS)_5]^{2\ominus}$ and $[Tc(NO)(NCS)_6]^{3\ominus}$.

Tetrabutylammonium salt: [90386-75-7].
Red cryst. Sol. Me_2CO. Paramagnetic (low-spin d^5); molar conductivity in MeCN is that of a 1:1 salt.

Orvig, C. *et al*, *J. Labelled Compd. Radiopharm.*, 1981, **18**, 148 (*synth, ir, conductivity*)
Davison, A., *Technetium in Chemistry and Nuclear Medicine*, Ed. Deutsch, E. *et al*, Cortina International, Verona, 1983, 3.
Kirmse, R. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **518**, 210; 1989, **573**, 63 (*props, esr, halide exchange*)
Köhler, K. *et al*, *Z. Chem.*, 1986, **26**, 339 (*synth, esr*)

IC-002042

$Br_4NOs^{\ominus}$

Tetrabromonitridoosmate(*VI*)(1−)
[47999-84-8]

$[N{\equiv}OsBr_4]^{\ominus}$ (C_{4v})

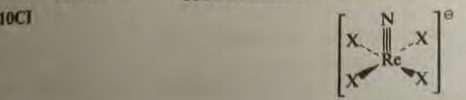
M 523.8 (ion)
Ph_4As salt: [42720-44-5].
Synth. by adding an aq. soln. of NaN_3 in conc. HBr to a mixt. of OsO_4 and $[AsPh_4]Cl$ in MeOH. Pink cryst. (MeCN). Sol. MeCN. Ir ν 1120, 270, 232 cm^{-1}.

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir, uv*)
Mahmoudi, S. *et al*, *Rev. Chim. Minér.*, 1978, **15**, 254 (*ir*)
Collison, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1812 (*cryst struct, uv*)
Nefedov, V.I. *et al*, *Dokl. Akad. Nauk SSSR*, 1986, **291**, 614 (*pe*)
Kravchanko, E.A. *et al*, *Koord. Khim.*, 1987, **13**, 1520 (*nqr*)

IC-002043

$Br_4NRe^{\ominus}$

Tetrabromonitridorhenate(*VI*)(1−)



X = Br

M 519.8 (ion)
Distorted sq. pyramid. Interatomic distances: Re≡N 162.0, Re—Br 247.7 pm. Ir $\nu_{Re{\equiv}N}$ 1099 cm^{-1}. For BBr_3 adduct, see (Boron tribromide) tetrabromonitridorhenate(*VI*)(1−), IC-000784.

Ph_4As salt: [83533-88-4].
Synth. from $AsPh_4[ReNCl_4]$ and BBr_3, followed by thermal cleavage of the resulting $AsPh_4[Br_4ReN(BBr_3)]$. Red-orange cryst. (CH_2Br_2).

Kaßitz, W. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **490**, 175 (*synth, ir, cryst struct*)

$Br_4NRu^{\ominus}$

IC-002044

Tetrabromonitridoruthenate(*VI*)(1−), 9Cl
[53149-54-5]

$[N{\equiv}RuBr_4]^{\ominus}$ (C_{4v})

M 434.6 (ion)
Prepd. by treating $[RuO_3Br_4]^{2\ominus}$ with $Na[N_3]$ in aq. HBr. Sol. MeCN, aq. HBr. Along with $[RuNCl_4]^{\ominus}$, $[RuNBr_4]^{\ominus}$ shows the largest quadrupole splittings yet obsd. for ^{99}Ru: the *six* component lines are almost resolved.

Tetrabutylammonium salt: Brown cryst.; diamagnetic.
Ph_4As salt: [42718-63-8].
Pink cryst.; diamagnetic. Ru≡N 158, Ru—Br 245.3 pm; angle: NRuBr 104.25°. Ir $\nu_{Ru{\equiv}N}$ 1088; ν_{Ru-Br} 304 cm^{-1}.

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth*)
Collin, R.J. *et al*, *J. Mol. Struct.*, 1973, **19**, 531 (*ir, raman*)
Gibb, T.C. *et al*, *Chem. Phys. Lett.*, 1974, **29**, 379 (*mössbauer*)
Collison, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1820 (*cryst struct, uv*)

IC-002045

$Br_4NTc^{\ominus}$

Tetrabromonitridotechnetate(*VI*)(1−)
[105059-13-0]

$[N{\equiv}TcBr_4]^{\ominus}$

M 432.5 (ion)
Square pyramidal with axial N≡Tc. Synth. by N_2H_4 reduction of $TcO_4^{\ominus}/Br^{\ominus}$; by $N_3^{\ominus}$ reduction of $TcO_4^{\ominus}$ in conc. HBr; or from $TcNCl_4^{\ominus}$ + LiBr in Me_2CO. Starting material for synth. of complexes with $[Tc^{VI}{\equiv}N]^{3\oplus}$ core. Air-stable.

Tetrabutylammonium salt: [95012-29-6].
Brilliant blue cryst. (MeCN). Mp 202-203°.
Ph_4As salt: [95012-28-5].
Intense blue-black cryst. (MeCN). Sol. CH_2Cl_2. Mp 293-295° dec.

Kaden, L. *et al*, *Isotopenpraxis*, 1981, **17**, 174 (*synth*)
Baldas, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 2395; 1987, 1721 (*synth, ir, uv, esr*)
Baldas, J. *et al*, *Aust. J. Chem.*, 1985, **38**, 215 (*cryst struct*)
Baldas, J. *et al*, *Inorg. Chem.*, 1986, **25**, 150 (*synth, ir*)
Köhler, K. *et al*, *Z. Chem.*, 1986, **26**, 339 (*esr*)
Abram, U. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **544**, 167 (*esr*)

IC-002046

$Br_4N_2O_2Re^{\ominus}$

Tetrabromodinitrosylrhenate(1−), 11Cl

$[Re(NO)_2Br_4]^{\ominus}$

M 565.8 (ion)
Octahedral.

cis-form
Re—Br 251-254, Re—N 180, 184 pm.

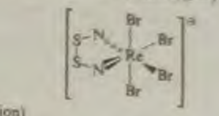
Ph_4P salt: Synth. from $PPh_4[Re(NO)_2Cl_4]$ and BBr_3. Dark red-brown powder.
Ph_4P salt, $2CCl_4$ solvate: [84151-08-6].
Dark red-brown cryst.

Mronga, V.N. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **491**, 237 (*synth, ir, cryst struct, props*)

IC-002047

$Br_4N_2ReS_2^{\ominus}$

Tetrabromo(disulfur diamidato(4−)-*N,N'*)rhenate(1−), 11Cl
Tetrabromo(disulfur dinitrido)rhenate(1−)



M 597.9 (ion)
Ph_4P salt: [105034-14-8].
Synth. from $PPh_4[ReCl_4(NSCl)_2]$ and $BrSiMe_3$. Black cryst. (CH_2Br_2).

Conradi, E. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **559**, 39 (*synth, ir, cryst struct, props*)

IC-002048

Br_4Nb

Niobium bromide ($NbBr_4$), 11Cl
Niobium tetrabromide
[13842-75-6]

$NbBr_4$

M 412.5
Struct. not known. Synth. by reduction of $NbBr_5$ with Nb in a temp. gradient of 410-350° or by heating $NbBr_3$ and $NbBr_5$ in a sealed tube. Dark brown solid, readily oxidised in air. Disprop. to $NbBr_3$ + $NbBr_5$. Diamagnetic.

Schaefer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **311**, 134, 139 (*synth*)
McCarley, R.E. *et al*, *Inorg. Chem.*, 1963, **2**, 540 (*synth, struct*)
Berdonosov, S.S. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 1338 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1448 (*synth*)

IC-002049

$Br_4Ni^{2\ominus}$

Tetrabromonickelate(*II*)(2−), 9Cl, 8Cl
[15954-87-7]

$[NiBr_4]^{2\ominus}$

M 378.3 (ion)
Tetrahedral struct. Many salts known, most stable being those with large cations. Paramagnetic.

Bis-Et_4N salt: [1185-60-0].
Blue deliquescent needles. Sol. MeCN, $MeNO_2$.
Bis-tetrabutylammonium salt: [7270-22-6].
Blue solid.

[35063-90-2]

Gill, N.S. *et al*, *J. Chem. Soc.*, 1959, 3997 (*synth, uv, elec cond*)
Goodgame, D.M.L. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 4161 (*uv-vis*)
Sabatini, A. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 17 (*ir*)
Inorg. Synth., 1967, **9**, 136 (*synth*)
Inman, G.W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 721 (*magnetism*)
Escard, J. *et al*, *Inorg. Chem.*, 1974, **13**, 895 (*pe*)

IC-002050

Br_4Np

Neptunium(*IV*) bromide ($NpBr_4$)
Neptunium tetrabromide
[15608-32-9]

$NpBr_4$

M 556.6
Isostructural with UBr_4 with 8-coord. Np. Synth. from Np + Br_2 (*in vacuo* at 425°) or from NpO_2 + $AlBr_3$ (350°). Moisture-sensitive red-brown solid. Sol. Me_2CO, $MeNO_2$, EtOH. Mp 464°. Bp 400° *in vacuo*.

Fried, S. *et al*, *J. Am. Chem. Soc.*, 1948, **20**, 3539 (*synth*)
U.S. Pat., 2 578 410, (1952); *CA*, **46**, 3716 (*synth*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1970, 476 (*synth, struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1267 (*synth*)

$Br_4ORe^{\ominus}$ IC-002051

Tetrabromorhenate(*V*)(1 –)
Oxotetrabromorhenate(V)(*1* –)

$[O{=}ReBr_4]^{\ominus}$ (C_{4v})

M 521.8 (ion)
Probably square pyramidal with apical oxygen. Salts hydrol. instantly in H_2O and slowly in moist air. Ion readily adds neutral ligands eg. MeCN, Ph_3P and Py.

Cs salt:
Br_4CsORe M 654.7
Synth. analogously to Ph_4As salt. Red-orange platelets (conc. HBr); dried at 80° *in vacuo*. Sl. sol. 48% HBr.
Et_4N salt: Synth. from $KReO_4$ by treatment with Zn in conc. H_2SO_4, followed by 48% HBr aq. and Et_4NBr. Red cryst. + H_2O (Me_2CO). Sol. Me_2CO, MeCN. Insol. hydrocarbons, alcohols, ethers and $CHCl_3$.
Ph_4As salt: [14853-12-4].
Synth. from $KReO_4$ by treatment with Zn in conc. H_2SO_4/MeOH, followed by 48% HBr and Ph_4AsBr. Coral-red cryst. (MeCN); dried at 80° *in vacuo*. Sol. Me_2CO, alcohols, MeCN, $CHCl_3$, THF. Insol. hydrocarbons, Et_2O and 48% HBr.

Cotton, F.A. *et al*, *Inorg. Chem.*, 1966, **5**, 9 (*synth, ir, uv, struct, props*)
Davison, A., *Inorg. Chem.*, 1980, **19**, 1988.
McDonell, A.C. *et al*, *Aust. J. Chem.*, 1983, **36**, 253.

Br_4ORe IC-002052

Rhenium(*VI*) bromide oxide ($ReBr_4O$)
Rhenium tetrabromide oxide. Tetrabromooxorhenium(VI)
[23601-08-3]

$ReOBr_4$ (C_{4v})

M 521.8
Believed to be molecular, isostructural with $ReOCl_4$. Synth. by (i) reaction of Re with SO_2 and Br_2, (ii) reaction of ReO_2 with Br_2, (iii) reduction of NH_4ReO_4 by NaBr in conc. H_2SO_4 followed by toluene extraction of $ReOBr_4$. Low melting blue-black solid. Ir ν_{ReO} 1005 cm^{-1}.

Colton, R., *J. Chem. Soc.*, 1962, 2078 (*synth*)
Edwards, D.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 145 (*synth, uv, ir, magnetism*)
Borisova, L.V. *et al*, *Inorg. Chim. Acta*, 1981, **54**, L233 (*synth, uv, raman, ms*)

$Br_4OTa^{\ominus}$ IC-002053

Tetrabromooxotantalate(*V*)(1 –), 11Cl

$[TaOBr_4]^{\ominus}$

M 516.5 (ion)
Nitrosyl salt: [87808-69-3].
Br_4NO_2Ta M 546.5
Synth. from NO[$TaOCl_4$] and BBr_3 at r.t. Red solid.

Dehnicke, K. *et al*, *Chem.-Ztg.*, 1983, **107**, 247 (*synth*)

$Br_4OTc^{\ominus}$ IC-002054

Tetrabromooxotechnetate(*V*)(1 –)
[73953-02-3]

$[O{=}TcBr_4]^{\ominus}$ (C_{4v})

M 434.5 (ion)
Synth. by reaction of $KTcO_4$ with 48% HBr at r.t. Valuable synthetic starting material for complexes with $TcO^{3\oplus}$ core. Water-sensitive (gives TcO_2 aq. + $TcO_4^{\ominus}$); also reacts with other donor solvs. May crystallise in the hydrated form $[TcOBr_4(OH_2)]^{\ominus}$ e.g. in $Et_4N^{\oplus}$ salt.
Tetrabutylammonium salt: [73953-03-4].
Green-yellow plates (CH_2Cl_2/hexane). Sol. CH_2Cl_2, MeCN, Me_2CO.

[92622-23-6]

Thomas, R.W. *et al*, *Inorg. Chem.*, 1980, **19**, 2840 (*synth, props, ir, uv, exafs*)
Preetz, W. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1355 (*synth, uv, ir*)
Gerasimov, V.N. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1982, **266**, 148 (*pe*)
Baran, E.J. *et al*, *Z. Naturforsch., A*, 1983, **38**, 563 (*ir*)
Thomas, R.W. *et al*, *Inorg. Chem.*, 1985, **24**, 1472 (*synth, ir, exafs*)
Mantegazzi, D. *et al*, *Inorg. Chim. Acta*, 1989, **167**, 195 (*props, Et_4N salt struct*)

$Br_4OV^{\ominus}$ IC-002055

Tetrabromooxovanadate(*V*)(1 –), 11Cl
Oxotetrabromovanadate(V)(*1* –)

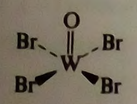
$[O{=}VBr_4]^{\ominus}$ (C_{4v})

M 386.5 (ion)
Square pyramidal. Interatomic distance: V–O 155 pm.
Ph_4P salt: [83343-82-2].
Synth. from Ph_4PBr and $VOBr_3$ in CH_2Br_2. Dark violet solid.

Müller, U. *et al*, *Z. Naturforsch., B*, 1982, **37**, 699 (*synth, cryst struct, ir*)

Br_4OW IC-002056

Tungsten(*VI*) bromide oxide (WBr_4O)
Tungsten tetrabromide oxide. Tetrabromooxotungsten(VI)
[13520-77-9]



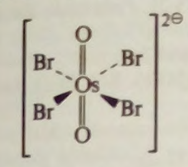
M 519.4
Square pyramidal struct. Synth. e.g. from WO_3 + CBr_4; WO_3-carbon mixt. + Br_2; WO_2—W mixt. with Br_2; WBr_6 + SO_2(l), WBr_6 + WO_3 at 100-150°; WO_3 + BBr_3. V. hygroscopic. dark purple-black or dark brown needles, or black lustrous solid. Rapidly dec. in air or H_2O. Sol. dioxan (→ yellow soln.), Me_2CO (→ green soln.); sol. RCN, R_2O, R_2S. Mp 277° (273-276°). $Subl._{0.5}$ 168-172°, Bp 327° (322°).

Lappert, M.F. *et al*, *J. Chem. Soc. A*, 1967, 129 (*synth*)
Fowles, G.W.A. *et al*, *J. Chem. Soc. A*, 1967, 671 (*synth, ir, complexes*)
Ward, B.G. *et al*, *Inorg. Chem.*, 1968, **7**, 2569 (*ir*)
Crouch, P.C. *et al*, *J. Chem. Soc. A*, 1969, 2412 (*synth*)
Singleton, D.L. *et al*, *Inorg. Chem.*, 1972, **11**, 1208 (*ms*)
Inorg. Synth., 1973, **14**, 109 (*synth*)

Kaposi, O. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1809 (*ms*)
Levason, W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 2501 (*synth, ir, uv*)
Shishkin, N.Ya. *et al*, *J. Mol. Struct.*, 1981, **73**, 249 (*ed*)
Müller, U., *Acta Crystallogr., Sect. C*, 1984, **40**, 915 (*cryst struct*)

$Br_4O_2Os^{2\ominus}$ IC-002057

Tetrabromodioxoosmate(*VI*)(2 –)

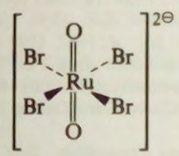


M 541.8 (ion)
trans-Octahedral.
Di-K salt: [22827-14-1].
Synth. from OsO_4 in KOH soln. and HCl. Raman $\nu_{Os-O_2\ sym}$ 899s; ν_{Os-Br} 193, 182 cm^{-1}.
Di-Cs salt: [22827-15-2].
Ir $\nu_{MO_2^{as}}$ 842vs; δ_{MO_2} 295s; ν_{Os-Br} 220w cm^{-1}.

Wintrebert, L. *et al*, *Ann. Chim. Phys.*, 1903, **28**, 15 (*synth*)
Griffith, W.P., *J. Chem. Soc. A*, 1969, 211 (*ir, raman*)
Hanuza, J. *et al*, *Acta Phys. Pol. A*, 1972, **42**, 537 (*ir*)
Jezowska-Trzebiatowska, B. *et al*, *Acta Phys. Pol. A*, 1980, **38**, 563 (*ir*)

$Br_4O_2Ru^{2\ominus}$ IC-002058

Tetrabromodioxoruthenate(*VI*)(2 –)



M 452.6 (ion)
trans-Octahedral anion.
Di-Cs salt: [31453-70-0].
Prepd. by treating a soln. of RuO_4 in CCl_4 with a soln. of CsBr in aq. HBr at 0°. Brown crystalline diamagnetic salt. Ir ν_{RuO_2} 825, 821 cm^{-1}.
[40580-97-0]

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)

$Br_4O_2U^{2\ominus}$ IC-002059

Tetrabromodioxouranate(*VI*)(2 –)
[18701-97-8]

$[UO_2Br_4]^{2\ominus}$

M 589.6 (ion)
trans-Octahedral anion.
Di-K salt: [64175-10-6].
$Br_4K_2O_2U$ M 667.8
Orange cryst. Sol. H_2O, HBr (aq.).
Di-Rb salt: [89189-90-2].
$Br_4O_2Rb_2U$ M 760.5
Orange cryst. + H_2O.
Di-Cs salt: [18324-47-5].
$Br_4Cs_2O_2U$ M 855.4
Pale orange hygroscopic prisms. Ir ν_{U-O} 925, 917 cm^{-1} (mull); raman ν_{U-O} 834 cm^{-1}.
Di-NH_4 salt: [65484-90-4].
$Br_4H_8N_2O_2U$ M 625.7
Orange cryst. + $2H_2O$. Sol. $MeNO_2$.
Bis-Me_4N salt: [52441-82-4].
Cryst. Raman ν_{U-O} 869 (soln); 832 cm^{-1} (solid).
Bis-tetrapropylammonium salt: [53140-36-6].
Brown cryst.
Bis-tetrabutylammonium salt: [65209-35-0].
Brown cryst.
Bis-Ph_4P complex: [57902-98-4].
Yellow cryst. + $2CH_2Cl_2$.
Bis(4,6-dimethyl-3-thioxo-3H-1,2-dithiolo[4,5-c]pyridinium) salt: [102539-11-7].
$C_{16}H_{10}Br_4N_2O_2S_6U$ M 1012.3
Orange-brown cryst. (plates). Sol. MeCN.

Ellert, G.V. *et al*, *Zh. Neorg. Khim.*, 1965, **10**, 1572; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 858 (*synth*)
Newberry, J.E., *Spectrochim. Acta, Part A*, 1969, **25**, 1699 (*ir*)
Mikhailor, Yu.N. *et al*, *Zh. Neorg. Khim.*, 1971, **16**, 2512; *Russ. J. Inorg. Chem. (Engl. Transl.)*, **16**, 1340 (*synth*)
Di Sipio, L. *et al*, *Cryst. Struct. Commun.*, 1972, **6**, 723; 1974, **3**, 297, 301 (*cryst struct*)
Ohwada, K. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1601 (*ir*)
Di Sipio, L. *et al*, *Inorg. Chim. Acta*, 1979, **37**, 149 (*cryst struct, uv-vis*)
Flint, C.D. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1982, **78**, 103 (*synth*)
Flint, C.D. *et al*, *Mol. Phys.*, 1983, **50**, 625 (*ir, raman, uv-vis, luminescence*)
Tanner, P.A., *J. Chem. Soc., Faraday Trans. 2*, 1984, **86**, 365 (*luminescence, ir, raman*)
Conradi, F. *et al*, *Chem. Ber.*, 1986, **119**, 2582 (*cryst struct*)
Van den Bossche, G. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 383 (*synth, cryst struct*)
Böhrer, R. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **558**, 119 (*synth, cryst struct*)

Br_4Os IC-002060

Osmium(*IV*) bromide ($OsBr_4$)
Osmium tetrabromide
[59201-52-4]

$OsBr_4$

M 509.8
It is not known whether Form I and Form II are identical. Osmium octahedrally coord. Form I synth. by reaction of the elements at 20 atm. of bromine at 450-470°; Form II by reaction of HBr and EtOH on OsO_4 under reflux followed by intensive drying. Black cryst. (Form I); black solid (Form II). Insol. in H_2O, mineral acids. Mp 350° dec. Dec. at 350° to $OsBr_3$ and Br_2.

Hepworth, M.A. *et al*, *J. Chem. Soc.*, 1954, 4269 (*synth*)
Semenov, I.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 111 (*synth, props, cryst struct*)
Thiele, G. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **530**, 178 (*cryst struct*)

$Br_4P^{\oplus}$ IC-002061

Tetrabromophosphonium
Tetrabromophosphorus(1+), 9Cl
[15099-42-0]

$[PBr_4]^{\oplus}$ (T_d)

M 350.5 (ion)
Chloride: [39118-22-4]. *Tetrabromophosphonium chloride*
Br_4ClP M 386.0
Yellow powder. Orthorhombic.
Bromide: see *Phosphorus bromide (PBr_5)*, IC-002118
Tribromide: see *Tetrabromophosphonium tribromide*, IC-002205
Tetrabromoborate: [51826-56-3].

BBr_4P M 681.0
Synth. from PBr_5 + BBr_3 in EtBr. Yellow solid. Tetrahedral anion.
Dibromoiodate: [17978-65-3].
Br_4IP M 637.3
Wine red cryst.
Hexafluorophosphate. [12514-48-6].
Tetrabromiphosphonium hexafluorophosphate
$Br_4F_6P_2$ M 495.5
White, unstable, cryst. powder. Dec. in soln. in non-polar solvs. → PBr_3, Br_2PF_3. Subl. 135° dec.
Trichloride: [118968-32-4].
Br_4Cl_3P M 456.9
Synth. from PCl_3 + Br_2 or PCl_3 + PBr_3. Orange cryst. (CCl_4). Non-conductor in solid state or in soln. in C_6H_6, CCl_4 or CS_2. Conductor when molten, or in soln. in $PhNO_2$ or MeCN.

Dhamelincourt, P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1971, **272**, 124 (*hexafluorophosphate*)
Gabes, W. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1972, **91**, 1367 (*chloride, raman, cryst struct*)
Finch, A. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1863 (*synth, raman, P-31 nmr*)
Rafaeloff, R. *et al, Spectrochim. Acta, Part A*, 1974, **30**, 1305 (*synth, raman*)
Dillon, K.B. *et al, Spectrochim. Acta, Part A*, 1974, **30**, 1873 (*B-11 nmr*)
Dillon, K.B. *et al, Polyhedron*, 1983, **2**, 641 (*P-31 nmr*)
Shamir, J. *et al, J. Raman Spectrosc.*, 1986, **17**, 463 (*synth, ir, raman*)
Dillon, K.B. *et al, Polyhedron*, 1988, **7**, 1725 (*trichloride, synth, raman, P-31 nmr, struct*)

IC-002062

Br_4P_2
Hypodiphosphorous tetrabromide, 9CI
Tetrabromodiphosphine. Tetrabromodiphosphorus(III). Tetrabromodiphosphane
[24856-99-3]

Br_2PPBr_2

M 381.5
Synth. from PBr_3 + R_4NI; or from PBr_3 by neutron irradiation. Easily hydrol. → P_2H_4.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 491 (*rev, bibl*)
Teague, J.L. *et al, Radiochim. Acta*, 1969, **11**, 57.
Dillon, K.B. *et al, Inorg. Nucl. Chem. Lett.*, 1981, **17**, 201 (*synth, P-31 nmr*)

IC-002063

Br_4Pa
Protactinium(*IV*) bromide ($PaBr_4$)
Protactinium tetrabromide
[13867-42-0]

$PaBr_4$

M 550.6
Possesses the UCl_4 struct. with 8-coord. Pa. Synth. from $PaBr_5$ + H_2 or Al at 400°. Orange-red solid. Sol. MeCN, EtOH, Me_2CO.

Brown, D. *et al, J. Chem. Soc. A*, 1967, **719**; 1971, 908 (*synth, cryst struct*)
Brown, D. *et al, Nature (London)*, 1969, **217**, 738 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1178 (*synth*)

IC-002064

$Br_4Pd^{2\ominus}$
Tetrabromopalladate(*II*)(2−)
[14127-70-9]

$[PdBr_4]^{2\ominus}$ (D_{4h})

M 426.0 (ion)
Dark red-brown ion.
Di-K salt: [13826-93-2]. *Potassium tetrabromopalladate* (K_2PdBr_4)
Br_4K_2Pd M 504.2
Dark red cryst. (HBr). Sol. H_2O. Isomorphous with K_2PtCl_4.
▷ RT3358000.
Di-Rb salt: [15654-53-2].
Br_4PdRb_2 M 596.9
Brown solid.
Di-Cs salt: [15654-54-3].
Br_4Cs_2Pd M 691.8
Brown solid.
Tetraamminepalladium(2+) salt: [15278-85-0].
$Br_4H_{12}N_4Pd_2$ M 600.5
Dichroic red-brown solid. Magnus-type struct.; Isom. to $Pd(NH_3)_2Br_2$ on heating to 190°.
Bis-Et_4N salt: [70468-65-4].
Exhibits antitumour activity in mice. Red cryst. Sol. MeCN, Ac_2O, $PhNO_2$, $MeNO_2$, MeOH, Me_2CO.
Bis-tetrabutylammonium salt: [54189-55-8].
Formed on fusion of $[Pd_2Br_6]^{2\ominus}$ with excess $[Bu_4N]Br$. Brown solid.

Biilmann, E. *et al, Ber.*, 1903, **36**, 1565 (*synth*)
Harris, C.M. *et al, J. Chem. Soc.*, 1959, 1505 (*synth, uv-vis*)
Hendra, P.J., *J. Chem. Soc. A*, 1967, 1298 (*raman, ir*)
Perry, C.H. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 1137 (*ir*)
Hirashi, J. *et al, Spectrochim. Acta, Part A*, 1968, **24**, 819 (*ir*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1479 (*ir, synth, raman*)
Martin, D.A. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2538 (*cryst struct*)
Bosworth, Y.M. *et al, Inorg. Chem.*, 1975, **14**, 171 (*raman, uv-vis*)
Kukushkin, Yu.N. *et al, Zh. Neorg. Khim.*, 1976, **21**, 2721; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1497 (*reaction*)

IC-002065

Br_4Po
Polonium(*IV*) bromide ($PoBr_4$)
Polonium tetrabromide

$PoBr_4$

M 529.5
Synth. by reaction of Po + Br_2 at 200-250°. Bright-red solid. Hygroscopic and readily hydrol. Sol. EtOH. Sl. sol. Br_2. Mp 330° (in Br_2 vap.). Bp_{200} 360°.

Bagnall, K.W. *et al, J. Chem. Soc.*, 1956, 3959 (*synth*)
Bagnall, K.W., *Adv. Inorg. Chem. Radiochem.*, 1962, **4**, 197 (*rev*)
Bagnall, K.W., *The Chemistry of Se, Te, Po*, Elsevier, 1966, 104 (*rev*)

IC-002066

$Br_4Pt^{2\ominus}$
Tetrabromoplatinate(*II*)(2−), 8CI
[14493-01-7]

$[PtBr_4]^{2\ominus}$

M 514.6 (ion)

Probable square planar struct. Many other salts with organic or complex cations known. Many studies of reaction mechanisms. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + $Br^{\ominus}$ or Hexabromoplatinate(*IV*)(2−), IC-002173 + N_2H_4. Useful starting material.
Di-Na salt: [21246-31-1]. *Sodium tetrabromoplatinate*(II) (Na_2PtBr_4)
Br_4Na_2Pt M 560.6
Probably brown solid. Probably sol. H_2O.
Di-K salt: [13826-94-3]. *Potassium tetrabromoplatinate*(II) (K_2PtBr_4)
Br_4K_2Pt M 592.8
Commercially available. Brown solid. Sol. H_2O. The dihydrate is probably identical.
▷ TP1830000.
[65531-65-9]

Duddell, D.A. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 879 (*ir, raman*)
Adams, D.M. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 947 (*ir*)
Inorg. Synth., 1979, **19**, 2 (*synth*)
Kerrison, S.J.S. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 2363 (*Pt-195 nmr*)
Isci, H. *et al, Inorg. Chem.*, 1984, **23**, 1565 (*uv, mcd*)

IC-002067

Br_4Pt
Platinum(*IV*) bromide ($PtBr_4$), 9CI
Platinum tetrabromide
[68938-92-1]

$PtBr_4$

M 514.6
Struct. not determined, prob. contains polymeric chains of $PtBr_6$ units. Synth. from Platinum, IC-021805 + HBr (aq.) + Br_2. Dark red solid. Sol. EtOH, Et_2O; sl. sol. H_2O. Dec. at 180°.

Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1615.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1713 (*synth*)

IC-002068

Br_4Re
Rhenium(*IV*) bromide ($ReBr_4$), 9CI
Rhenium tetrabromide
[36753-03-4]

$ReBr_4$

M 505.8
Believed to be isostructural with γ-$ReCl_4$. Synth. from $ReCl_5$ and BBr_3. Black powder.

Colton, R. *et al, Chem. Ind. (London)*, 1959, 1314.
Müller, H. *et al, Inorg. Nucl. Chem. Lett.*, 1972, **8**, 413 (*synth, struct*)

IC-002069

Br_4Ru
Ruthenium(*IV*) bromide ($RuBr_4$)

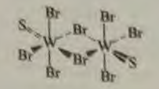
$RuBr_4$

M 420.6
Unknown at present.

Seddon, E.A. *et al, The Chemistry of Ruthenium*, Elsevier, Amsterdam, 1984, 92.

IC-002070

Br_4SW
Tungsten(*VI*) bromide sulfide ($WSBr_4$)
[27388-80-3]



dimer

M 535.5
Square pyramidal units weakly associated to give dimer in solid state. Monomeric in gas phase. Synth. from Sb_2S_3 and WBr_6 at 140°.
Dimer: Di-μ-bromohexabromodithioxoditungsten(VI)
$Br_4S_2W_2$ M 1071.0
V. air-sensitive dark green cryst. Subl. *in vacuo*. Ir *v* 555, 395, 346, 250 cm^{-1}.

Drew, M.G.B. *et al, J. Chem. Soc. A*, 1970, 2815 (*struct*)
Britnell, D. *et al, J. Chem. Soc., Chem. Commun.*, 1970, 608 (*synth, ir*)
Britnell, D. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 2191 (*synth*)
Jones, P.J. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2625 (*ir, uv-vis, struct*)

IC-002071

$Br_4Sb^{\ominus}$
Tetrabromoantimonate(*III*)(1−), 8CI
[20057-68-5]

$[SbBr_4]^{\ominus}$

M 441.3 (ion)
Salts obt. from $R_4N^{\oplus}Br^{\ominus}$ + $SbBr_3$ in $MeOH/MeNO_2$.
Me_4N salt: [30454-64-9].
Orange-red soln. in $SOBr_2$.
Et_4N salt: [30454-65-0].
Orange-red soln. in $SOBr_2$.
Tetrabutylammonium salt: [22364-15-4].
Lemon solid or cryst. (CH_2Cl_2). Insol. MeOH. Mp 109-110°.
H compd.: see *Hydrogen tetrabromoantimonate*(III)(1−), *IC-002023*

Gmelin Handbook Inorg. Chem., Syst. No. 18, 1949, 482 (*rev, bibl*)
Ahlijah, G.Y. *et al, J. Chem. Soc. A*, 1970, 326 (*synth, ir, raman*)
Paul, R.C. *et al, J. Indian Chem. Soc.*, 1970, **47**, 635 (*formn*)
Kolditz, L. *et al, Z. Anorg. Allg. Chem.*, 1973, **395**, 207 (*uv*)
Ballard, J.G. *et al, Can. J. Chem.*, 1974, **52**, 2375 (*mössbauer*)
Leroy, M.J.F. *et al, Bull. Soc. Chim. Fr.*, Part 1, 1979, 120 (*synth, raman*)
Kapoor, R. *et al, Can. J. Chem.*, 1987, **65**, 1195 (*synth*)

IC-002072

Br_4Se
Selenium(*IV*) bromide ($SeBr_4$)
Selenium tetrabromide
[7789-65-3]

$[SeBr_3]^{\oplus}Br^{\ominus}$ or $SeBr_4$ (tbp, with equatorial lone pair)

M 398.5
Exists in stable α and metastable β forms. Synth. from Se + Br_2. Orange-red solid, hygroscopic and readily hydrol. Readily dissociates to Br_2 + $SeBr_2$. Sol. org. solvs., HSO_3Cl. Mp 75° dec. Bp 123° (sealed tube). Forms M_2SeBr_6 with MBr.

Gmelin Handbook Inorg. Chem., Syst. No. 10, 1949, 150; 1984, **B2**, 238 (*bibl*)
George, J.W. *et al, Inorg. Chem.*, 1967, **6**, 903 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 419 (*synth*)

Br_4SeW IC-002073

Tungsten(*VI*) bromide selenide (WBr_4Se)

[54769-62-2]

$[WSeBr_4]$

M 582.4
Isostructural with $WSBr_4$ (dimer). Monomeric in gas phase. Synth. from Sb_2Se_3 and WBr_6 at 120°.
Dimer: Di-μ-bromidotetrabromidodiselenidoditungsten(VI)
V. air- and moisture-sensitive red solid.

Brittnell, D. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 2191 (*synth*)
Jones, P.J. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2625 (*ir, uv-vis, struct*)

Br_4Si IC-002074

Silicon bromide ($SiBr_4$)

Silicon tetrabromide. Tetrabromosilane

[7789-66-4]

$SiBr_4$ (T_d)

M 347.7
Colourless fuming liq. (cubic solid); hydrol. by H_2O, H_2SO_4. Mp 5.4°, Fp −12°. Bp 154°.

Kurdyumov, G.M. *et al, Izsled. Obl. Neorg. Tekhnol.*, 1972, 351 (*synth*)
Maciaiowicz, A. *et al, Pr. Inst. Technol. Elektron. (Warsaw)*, 1973, 6, 17 (*synth*)
Andrews, S.P. *et al, J. Chem. Res. (S)*, 1978, 94 (*ir*)
Olah, G.A. *et al, Organometallics*, 1982, **1**, 1485 (*Si-27 nmr*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3024.

Br_4Sn IC-002075

Tin(*IV*) bromide ($SnBr_4$)

Tin tetrabromide. Tetrabromostannane, 9CI. Stannic bromide

[7789-67-5]

$SnBr_4$

M 438.3
Synth. by direct bromination of tin. Hygroscopic cryst., fumes in air. Dec. in water. Mp 31°. Bp 202°.

▷ XP8300000.

Brand, P. *et al, Acta Crystallogr.*, 1963, **16**, 446 (*cryst struct*)
Knowles, D.J. *et al, J. Phys. Chem.*, 1970, **74**, 3642 (*ms*)
Druce, P.M. *et al, J. Chem. Soc. A*, 1971, 3595 (*synth*)
Debye, N.W.G. *et al, J. Chem. Phys.*, 1974, **61**, 4770 (*mössbauer*)
Gospodinov, G.G. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1977, **22**, 1559 (*synth*)
Andrews, S.P. *et al, J. Chem. Res. (S)*, 1978, 94 (*ir, raman*)
Colton, R. *et al, Inorg. Chim. Acta*, 1982, **61**, 1 (*Sn-119 nmr*)

Br_4Ta IC-002076

Tantalum bromide ($TaBr_4$), 11Cl

Tantalum tetrabromide

[13842-76-7]

$TaBr_4$

M 500.5
Struct. not known. Synth. by reducing $TaBr_5$ with eg. Ta or Al in a temp. gradient. Dark solid, readily oxidised in air. Mp 392° (incongr.). Disproportionates above 400°. Diamagnetic. $\Delta H_f°$ −520 kJ mol^{-1}.

McCarley, R.E. *et al, Inorg. Chem.*, 1963, **2**, 547; 1965, **4**, 1486 (*synth, phase diagram*)

Berdonosov, S.S. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 1336 (*synth, struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1455 (*synth*)
Woodland, A.D., *Can. J. Chem.*, 1980, **58**, 938 (*heat of format*)

$Br_4Tc^{2\ominus}$ IC-002077

Tetrabromotechnetate(*II*)(2−)

$[TcBr_4]^{2\ominus}$ (T_d)

M 418.5 (ion)
cis-Bis(2,2'-bipyridine-N,N')bromonitridotechnetium(V)(1+) salt: [121827-71-2].
$C_{40}H_{32}Br_4N_{10}Tc_2$ M 1428.9
Synth. by reaction of $[TcNBr_4]^{\ominus}$ with bipy in EtOH. Deep red solid + 0.5 MeOH (MeOH). Octahedral cation.

Archer, C.M. *et al, J. Chem. Soc., Chem. Commun.*, 1989, 375 (*cryst struct*)
Archer, C.M. *et al, Polyhedron*, 1989, **8**, 1879 (*synth*)

Br_4Tc IC-002078

Technetium(*IV*) bromide ($TcBr_4$)

Technetium tetrabromide. Tetrabromotechnetium(IV)

[74078-05-0]

$TcBr_4$

M 418.5
Synth. by successive evapn. of $HTcO_4$ in 40% HBr to dryness. Unstable red-brown solid; moisture-sensitive. Sol. Me_2CO.

Fergusson, J.E. *et al, Aust. J. Chem.*, 1970, **23**, 453 (*synth*)
Tsalas, S. *et al, Talanta*, 1980, **27**, 201 (*gc*)
Tsalas, S. *et al, Radiochim. Acta*, 1981, **29**, 217 (*thermodyn*)
Gmelin Handbook Inorg. Chem., Syst. No. 69 Suppl., 1983, **2**, 114 (*rev, bibl*)

Br_4Te IC-002079

Tellurium(*IV*) bromide ($TeBr_4$)

Tellurium tetrabromide

[10031-27-3]

$[TeBr_3]^{\oplus}Br^{\ominus}$ (solid state struct.)

M 447.2
Synth. from Te + Br_2. Yellow solid. Hygroscopic and readily hydrol. Dissociates as vap. to Br_2 + $TeBr_2$. Sol. $CHCl_3$, Et_2O, insol. CCl_4. Mp 363° (in Br_2 vap.). Bp 414-427°.

Schoemaker, C.B., *Acta Crystallogr.*, 1965, **18**, 296 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 434 (*synth*)

Br_4Th IC-002080

Thorium(*IV*) bromide ($ThBr_4$)

Thorium tetrabromide

[13453-49-1]

$ThBr_4$

M 551.6
Exists in α- and β-forms. Synth. from e.g. Th + Br_2 or Br_2 + ThO_2/C. Forms complexes with a range of donor ligands. Forms hydrates $ThBr_4.nH_2O$ (n = 7, 8, 10, 12). Hygroscopic white solid. Sol. H_2O. Mp 679° (610°). Bp 857° (725°). Can be sublimed *in vacuo* >600°.

α-form

Possesses the α-$TiCl_4$ struct. Dodecahedral about Ti.

β-form

Possesses the UCl_4 struct. Dodecahedral about Th.

Berzelius, J., *Pogg. Ann.*, 1829, **16**, 385 (*synth*)
Mossaz, B. *et al, Ann. Chim. Phys.*, 1897, **7**, 427 (*synth*)
Inorg. Synth., 1939, **1**, 51
Fischer, W. *et al, Z. Anorg. Allg. Chem.*, 1939, **242**, 161 (*synth*)
Brown, D. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 686 (*cryst struct*)
Mason, J.T. *et al, J. Less-Common Met.*, 1974, **35**, 331 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1139 (*synth*)
Malek, C.K. *et al, J. Mol. Struct.*, 1982, **83**, 201 (*raer*)
Guilhaumont, R., *Radiochim. Acta*, 1983, **32**, 129 (*rev*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 1129 (*complexes*)

Br_4Ti IC-002081

Titanium bromide ($TiBr_4$), 11Cl

Titanium tetrabromide

[7789-68-6]

$TiBr_4$

M 367.4
Tetrahedral in vapour phase and in the solid state (SnI_4 struct.). Ir of liq. also indicates a tetrahedral struct. Best synth. from Ti + Br_2 in a flow system at 300-600°. TiO_2 and C can be brominated at 600° or $TiCl_4$ caused to react with BBr_3. Ti also reacts with molten $PbBr_2$. Has been used extensively in catalysts, esp. for olefin polym. Amber yellow, readily hydrol. solid. There is a phase change at −15°. Sol. $CHCl_3$, CCl_4, Et_2O, EtOH. Mp 39°. Bp 230-238°. $\Delta H_f°$ −618 kJ mol^{-1}.

Brand, P. *et al, Z. Anorg. Allg. Chem.*, 1966, **348**, 257 (*cryst struct*)
Druce, P.M. *et al, J. Chem. Soc. A*, 1971, 3595 (*synth*)
Elias, H. *et al, Z. Anorg. Allg. Chem.*, 1972, **393**, 207 (*synth*)
Auge, O. *et al, Actual. Chim.*, 1977, 27 (*synth*)

$Br_4Tl^{3\ominus}$ IC-002082

Tetrabromothallate(*I*)(3−)

$[TlBr_4]^{3\ominus}$

M 523.9 (ion)
Synth. from TlBr and corresp. bromide salt of supporting cation in soln. Luminescent.

▷ V. toxic.

Scott, A.B. *et al, Inorg. Chem.*, 1962, **1**, 313 (*dissoc const*)
Curtice, R.E. *et al, Inorg. Chem.*, 1964, **3**, 1383 (*alkali halide complexes*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 881 (*synth*)

$Br_4Tl^{\ominus}$ IC-002083

Tetrabromothallate(*III*)(1−)

[15905-99-4]

$[TlBr_4]^{\ominus}$ (T_d)

M 523.9 (ion)
$TlBr_4^{\ominus}$ are arranged to form tunnels in which alkali metal ions and H_2O molecules located (c.f. zeolites). Obt. by slow evap. of aq. $TlBr_3$ and excess alkali metal bromide; or reaction of R_4NBr or R_4AsBr with $TlBr_3$ in non-aq. soln.

▷ Toxic.

K salt: [61129-43-9].

Br_4K_2Tl M 563.0
Synth. from $TlBr_3$ and KBr in aq. soln. Yellow cryst. + $2H_2O$.

[15698-65-7, 15698-88-5, 86593-30-8]

Spain, T.G., *Inorg. Chem.*, 1967, **6**, 589 (*ir*)
Glusker, J., *Acta Chem. Scand., Ser. A*, 1980, **34**, 157 (*synth, struct*)
Rotter, H.W. *et al, Z. Kristallorsch., B*, 1982, **37**, 995 (*synth, struct*)

Br_4Tl_2 IC-002084

Thallium(*I*) tetrabromothallate(*III*)

Thallium bromide (Tl_2Br_4). Thallium dibromide (mixed-)

[13453-28-6]

$Tl[TlBr_4]$

M 728.3
Synth. from TlBr + Br_2 in EtOH. Light beige orthorhombic cryst. Sol. HCl, sol. with dec. in oxidising acids, hydroxides; insol. H_2O, org. solvs. Forms solid solns. with Thallium(*I*) tetrachlorothallate(*III*), IC-017141 including compd. of composition TlClBr whose struct. resembles NiAs.

▷ Highly toxic.

Hazell, A.C. *et al, J. Chem. Soc.*, 1963, 3459 (*struct*)
Batsanov, S.S. *et al, Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1964, 91.
Thiele, G. *et al, Z. Anorg. Allg. Chem.*, 1975, **414**, 47.

Br_4U IC-002085

Uranium(*IV*) bromide (UBr_4)

Uranium tetrabromide

[13470-20-7]

UBr_4

M 557.6
Possesses layer struct. with pentagonal bipyramidal U. Synth. from U + Br_2/He at 650°, or from UO_3 + CBr_4 at 165°. V. air and moisture-sensitive brown monoclinic cryst. Sol. Me_2CO, EtOH. Mp 519° (516°). Bp 791° (761°). Reacts with O_2 → Uranium bromide oxide (UBr_2O_2). IC-001867 at 150°. With H_2 forms UBr_3 at 470°. Paramagnetic, μ_{eff} = 3.12μ_B (72-569K). Ir ν_{U-Br} 233 cm^{-1} (vapour).

Hönigschmid, O. *et al, Monatsh. Chem.*, 1915, **36**, 51 (*synth*)
Hönigschmid, O. *et al, Z. Anorg. Allg. Chem.*, 1936, **226**, 296 (*synth*)
Prigent, J., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1954, **238**, 102 (*synth*)
Douglas, R.M. *et al, Anal. Chem.*, 1957, **29**, 459 (*x-ray*)
Clifton, J.R. *et al, J. Chem. Phys.*, 1969, **51**, 224 (*electronic spec*)
Blair, A. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 3795 (*synth*)
Taylor, J.C. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 2664 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1214 (*synth*)
Korba, V.M., *Zh. Strukt. Khim.*, 1983, **24**, 172.

$Br_4V^{\ominus}$ IC-002086

Tetrabromovanadate(*III*)(1−), 8Cl

[15051-00-0]

$[VBr_4]^{\ominus}$

M 370.5 (ion)
May be tetrahedral based on uv-vis spectra but the low magnetic moment suggests an octahedral polymer.

Et_4N salt: [15636-55-2].

Synth. by adding $[Et_4N]Br$ to VBr_3 in MeCN and heating the product to remove MeCN. Brown-green solid. Paramagnetic, $\mu_{eff} = 2.41\mu_B$ (indep. of temp.).

Clark, R.J.H. *et al*, *J. Chem. Soc. A*, 1966, 1296 (*synth, ir, uv-vis*)
Gutman, V. *et al*, *Monatsh. Chem.*, 1967, **98**, 286 (*formn*)
Casey, A.T. *et al*, *Inorg. Chem.*, 1968, **7**, 1598 (*ir, uv-vis, magnetism*)

IC-002087

Br_4V^-

Vanadium(*IV*) bromide (VBr_4), 11Cl

Vanadium tetrabromide

[13595-30-7]

VBr_4 (T_d)

M 370.5
Tetrahedral in vapour according to electron diffraction data. Synth. by reaction of $VBr_3 + Br_2$ at 325°. Catalyst for graft copolymers. Purple solid, unstable above −23° slowly forming $VBr_3 + Br_2$.

McCarley, R.E. *et al*, *Inorg. Chem.*, 1964, **3**, 54 (*synth*)
Netherlands Pat., 6 606 141, (1966); *CA*, **66**, 66455p (*use*)
Spitsidinov, V.P. *et al*, *Zh. Strukt. Khim.*, 1967, **8**, 160; *CA*, **67**, 6485 (*ed*)
Ivashkevic, L.S. *et al*, *J. Mol. Struct.*, 1979, **51**, 217 (*ed*)

Br_4W IC-002088

Tungsten bromide (WBr_4)

Tungsten tetrabromide

[14055-81-3]

WBr_4

M 503.4
Prepd. by reduction of WBr_5 with Al metal. Black cryst.

McCarley, R.E. *et al*, *Inorg. Chem.*, 1964, **3**, 1232 (*synth*)

$Br_4Zn^{2\ominus}$ IC-002089

Tetrabromozincate(2−)

[16594-87-9]

$[ZnBr_4]^{2\ominus}$

M 385.0 (ion)
Many compds. containig this ion are known.

Morosin, B. *et al*, *Acta Crystallogr.*, 1959, **12**, 611, 744 (*cryst struct*)
Coates, G.E. *et al*, *J. Chem. Soc.*, 1964, 166 (*ir*)
Bird, B.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 741 (*uv*)
Macklin, J.W. *et al*, *Inorg. Chem.*, 1970, **9**, 821 (*raman*)
Asker, W.J. *et al*, *Aust. J. Chem.*, 1972, **25**, 2301 (*synth, nqr*)
Maciel, G.E. *et al*, *J. Phys. Chem.*, 1977, **81**, 263 (*Zn-67 nmr*)

Br_4Zr IC-002090

Zirconium bromide ($ZrBr_4$), 11Cl

Zirconium tetrabromide

[13777-25-8]

$ZrBr_4$

M 410.8
Tetrahedral in the gas phase but octahedral zig-zag chains in the solid state. Synth. by bromination of ZrO_2 + C at 560°, or by reaction of $ZrCl_4$ with BBr_3. Used as an absorber in artificial kidneys. Commercially available. Mp 450°. Subl. 250°. ΔH_f −760 kJ mol^{-1}.

Ammoniate: [97549-60-5].
Diamminetetrabromozirconium(IV).
Hexaamminetetrabromozirconium(IV)

At −30°, $ZrBr_4$ forms three adducts in liq. NH_3. At 20°, $ZrBr_4(NH_3)_6$ is stable but $ZrBr_4(NH_3)_2$ is stable at 200°. Four compositions known, $ZrBr_4(NH_3)_n$ where n = 2, 6, 12 or 17.

[97396-40-2]

Canterford, J.H. *et al*, *Halides of the Second and Third Row Transition Metals*, Wiley, New York, 1968 (*rev*)
Krebs, B. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **378**, 263 (*cryst struct*)
Druce, P.M. *et al*, *J. Chem. Soc. A*, 1971, 3595 (*synth*)
Girichev, G.V. *et al*, *Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1975, **18**, 1646; *CA*, **84**, 52478r (*ed*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1357 (*synth*)
Taylor, R.C. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 293 (*ir, raman*)
Boyle, E.L. *et al*, *Inorg. Chim. Acta*, 1985, **100**, 281 (*synth, deriv*)
Japan. Pat., 60 132 644, (1985); *CA*, **104**, 56466q (*use*)

$Br_5^{\ominus}$

Pentabromide(1−) IC-002091

[28712-15-4]

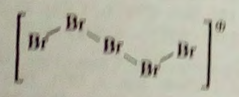
$[Br_5]^{\ominus}$

M 399.5 (ion)
Dark red in soln. Salts not isol. Dissociates in H_2O.

Hecquet, B. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1353 (*synth, raman*)
Rallo, F. *et al*, *J. Electrochem. Soc.*, 1972, **119**, 1471 (*synth*)
Bellucci, G. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 199 (*uv, formn const*)

$Br_5^{\oplus}$

Pentabromine(1+) IC-002092



M 399.5 (ion)
'Z-shaped' cation.

Tetrakis(fluorosulfato-O)aurate(1−): [72016-94-5].
$AuBr_5F_8O_{12}S_4$ M 992.7
Synth. from $Br_3[Au(SO_3F)_4]$ and Br_2 at 70°. Hygroscopic dark brown solid. Mp 65° dec.
Hexafluoroarsenate: [131906-72-4].
$AsBr_5F_6$ M 588.4
Synth. from $XeFAsF_6$ and Br_2 under an inert gas. Dark brown rectangular cryst.
Hexafluoroantimonate: [131906-73-5].
Br_5F_6Sb M 635.2
Synth. from $XeFSbF_6$ and Br_2 under an inert gas. Dark brown rectangular cryst.

Lee, K.C. *et al*, *Inorg. Chem.*, 1980, **19**, 119 (*synth, raman*)
Hartl, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1991, **30**, 328.

$Br_5Cd^{3\ominus}$ IC-002093

Pentabromocadmate(3−)

[85920-48-5]

$[CdBr_5]^{3\ominus}$

M 511.9 (ion)
Tri-Cs salt: [52581-59-6].
Br_5CdCs_3 M 910.6
Phase in the system CsBr-$CdBr_2$-H_2O. Cryst.

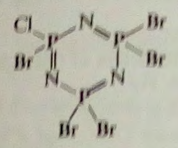
Heming, M. *et al*, *Z. Naturforsch., A*, 1981, **36**, 286 (*synth, cryst struct*)

$Br_5ClN_3P_3$ IC-002094

2,2,4,4,6-Pentabromo-6-chloro-2,2,4,4,6,6-hexahydro-1,3,5,2λ^5,4λ^5,6λ^5-triazatriphosphorine, 8Cl

Pentabromochlorocyclotriphosphonitrile.
Pentabromochlorocyclotriphosphazene. *2,2,4,4,6-Pentabromochloro-2λ^5,4λ^5,6λ^5-cyclotriphosphaza-1,3,5-triene.* *2,2,4,4,6-Pentabromo-6-chloro-1,3,5,2λ^5,4λ^5,6λ^5-triazatriphosphinine*

[15608-37-4]



M 569.9
Synth. from $PCl_5 + NH_4Br$. Solid. Mp 175°.

Rotzsche, H. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 687 (*gc*)
Steger, E. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 688 (*synth, ir*)
Engelhardt, G. *et al*, *Z. Naturforsch., B*, 1966, **21**, 1231 (*P-31 nmr*)
Coxon, G.E. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 381 (*synth, ir*)
Stahlberg, R. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2057 (*ir, raman*)
Coxon, G.E. *et al*, *J. Chem. Soc. A*, 1969, 358 (*ms*)

$Br_5ClOs^{2\ominus}$ IC-002095

Pentabromochloroosmate(*IV*)(2−)

[16920-03-9]

$[OsBr_5Cl]^{2\ominus}$

M 625.1 (ion)
A large number of the possible $[OsCl_nBr_{6-n}]^{2\ominus}$ complexes are known. On tempering a pure complex of the type $K_2[OsCl_nBr_{6-n}]$ (n = 1-5) to 110-200° all complexes with n = 0-6 are formed by intermolecular solid state interactions.

Joergensen, C.K. *et al*, *Z. Naturforsch., A*, 1967, **22**, 945 (*uv*)
Mueller, H., *Fresenius' Z. Anal. Chem.*, 1969, **247**, 145; 1983, **314**, 758 (*tlc, hplc*)
Prestz, W. *et al*, *Z. Anorg. Allg. Chem.*, 1974, **407**, 1; 1976, **420**, 97; 1981, **479**, 7 (*synth, uv, ir, kinetics*)
Urushiyama, A., *Chem. Lett.*, 1976, 1409 (*uv*)
Zerbe, H.D. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **479**, 17 (*kinetics*)

$Br_5Cr^{2\ominus}$ IC-002096

Pentabromochromate(*II*)(3−), 9Cl

[21910-40-7]

$[CrBr_5]^{3\ominus}$

M 451.5 (ion)
Bis-pyridinium salt: [32145-37-2].
Synth. by reaction of pyridinium acetate with $Cr(OAc)_3$ in AcBr/HOAc. Yellowish-green solid + HOAc.
[29794-90-9]

Hardt, H.-D. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **373**, 97 (*synth*)

$Br_5CrO^{2\ominus}$ IC-002097

Pentabromooxochromate(*V*)(2−), 9Cl

$[CrOBr_5]^{2\ominus}$

M 467.5 (ion)
Prepd. by reaction of $Cr_2O_7^{2\ominus}$ with satd. HBr.

2,2'-Bipyridinium(2+) salt: [57527-51-2].
Brownish-yellow solid.

Banerjea, A.K. *et al*, *Inorg. Chem.*, 1976, **15**, 488 (*synth, ir, esr*)

Br_5Cs_3Mn

Caesium manganese(*II*) bromide (Cs_3MnBr_5) IC-002098

Tricaesium bromide tetrabromomanganate(2−)

$Cs_3[MnBr_4]Br$

M 853.1
Contains tetrahedral $[MnBr_4]^{2\ominus}$, isomorphous with Cs_3MnCl_5. Synth. by heating stoichiometric amounts of CsBr and $MnBr_2$ at 650°. Cryst.

Amit, M. *et al*, *Isr. J. Chem.*, 1973, **11**, 749 (*synth, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, **C5**, 269 (*rev, bibl*)

$Br_5Cu^{3\ominus}$

Pentabromocuprate(*II*)(3−) IC-002099

[44236-91-1]

$[CuBr_5]^{3\ominus}$

M 463.0 (ion)
Trigonal bipyramidal anion.
Hexaamminechromium(3+) salt: [30482-48-5].
$Br_5CrCuH_{18}N_6$ M 617.2
Black cryst. Similar salts obt. for other $M(NH_3)_6^{3\oplus}$

Mori, M., *Bull. Chem. Soc. Jpn.*, 1960, **33**, 985 (*synth*)
Allen, G.C. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 281 (*uv*)
Goldfield, S.A. *et al*, *Inorg. Chem.*, 1971, **10**, 2604 (*cryst struct*)

$Br_5H_2IrO^{2\ominus}$ IC-002100

Aquapentabromoiridate(*III*)(2−), 10Cl

[62708-00-3]

$[IrBr_5(OH_2)]^{2\ominus}$

M 609.7 (ion)
Octahedral anion. Present in soln., not isol.

Kravisov, V.I. *et al*, *Elektrokhimiya*, 1970, **6**, 57317; *CA*, **73**, 29388 (*synth, kinetics*)
Melvin, W.S. *et al*, *Inorg. Chem.*, 1977, **16**, 2016 (*synth, kinetics*)

$Br_5H_2OPt^{\ominus}$ IC-002101

Aquapentabromoplatinate(*IV*)(1−), 8Cl

[17548-69-5]

$[(H_2O)PtBr_5]^{\ominus}$

M 612.6 (ion)
Salts not isol. Formed by hydrol. of $[PtBr_6]^{2\ominus}$. Subject of ligand substitution studies.

Davidson, C.M. *et al*, *Trans. Faraday Soc.*, 1965, **61**, 2462 (*formation, uv*)
Nikolaeva, N.M. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 650 (*formation*)
Elding, L.I. *et al*, *Inorg. Chim. Acta*, 1977, **22**, 201 (*substitutions*)

$Br_5H_2ORu^{2\ominus}$ IC-002102

Aquapentabromoruthenate(*III*)(2−), 10Cl

[74009-19-1]

$[Ru(OH_2)Br_5]^{2\ominus}$

M 518.6 (ion)

Claimed salts v. poorly characterised; no real evidence for formulation available. Now known to be salts of $[Ru_2Br_8]^{2\ominus}$.

Di-K salt: [62109-80-2].
Black cryst.
Di-Rb salt: Black cryst.
Di-Cs salt: Black cryst.

Howe, J.L., *J. Am. Chem. Soc.*, 1904, **26**, 942 (*synth*)
Gutbier, A. *et al*, *Z. Anorg. Allg. Chem.*, 1921, **115**, 225 (*synth*)
Fergusson, J.E. *et al*, *Aust. J. Chem.*, 1978, **31**, 497 (*reformulation*)

Br_2H_2Sb IC-002103

Dihydrogen pentabromoantimonate(*III*)(2−), 8CI
Pentabromoantimonic(III) acid

$H_2[SbBr_5]$

M 523.2
Salts prep. from Sb_2O_3 or $SbBr_3$ in HBr aq., + amine, HBr.
Bis-Me_2NH salt: [54205-68-4].
Yellow cryst. Mp 258-260°.
Bis-$EtNH_3$ salt: Yellow solid. Mp 249-250°.
Bis(2-chloropyridine) salt: [60362-47-2].
Orange cryst. Mp 121-130°. Struct. contains discrete $SbBr_5^{\ominus}$ anions (with tetragonal pyramidal geometry).
Bis-piperidine salt: Pale yellow solid. Stable in air. Insol. non-polar solvs. Mp 283° dec. Polymeric anion with zig-zag chains of $SbBr_6$ units.
Bis-aniline salt: [59450-19-0].
Yellow solid. Mp 180-181°.
Bis-benzylamine salt: [54331-35-0].
Yellow solid. Mp 170°.
Di-NH_3 salt: see *Diammonium pentafluoroantimonate(III) (2−), IC-018496*
[52279-36-4]

Gmelin Handbook Inorg. Chem., Syst. No. 18, 1949, 482 (*rev, bibl*)
Jha, N.K. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 2953; 1974, **36**, 1479; 1976, **38**, 401 (*synth*)
Hooper, M.A. *et al*, *Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)
Abdel-Rehim, H.A. *et al*, *Cryst. Struct. Commun.*, 1973, **2**, 45 (*cryst struct*)
Stewart, J.M. *et al*, *Inorg. Chem.*, 1974, **13**, 2767 (*synth, cryst struct*)
Carola, J.M. *et al*, *Cryst. Struct. Commun.*, 1976, **5**, 393 (*cryst struct*)
Cariati, F. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 801 (*synth, ir, raman*)
Leroy, M.J.F. *et al*, *Bull. Soc. Chim. Fr., Part I*, 1979, 120 (*synth, raman*)
Jagodzinski, P.W. *et al*, *J. Raman Spectrosc.*, 1980, **9**, 22 (*ir, raman*)
Okuda, T. *et al*, *Z. Naturforsch., A*, 1986, **41**, 319 (*nqr*)

Br_4Mo IC-002104

Molybdenum bromide ($MoBr_4$), 9CI
Molybdenum pentabromide
[14055-73-3]

$MoBr_4$

M 495.4
Prob. dimeric. Synth. from $MoCl_5$ + EtBr or PhBr in an atm. of oxygen-free Ar. Brown-black powder. Readily hydrol. in air.
Dimer: Di-μ-bromodecabromadimolybdenum
$Br_{10}Mo_2$ M 990.9

Golub, A.M. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 943, 1008 (*synth*)

$Br_5MoO^{2\ominus}$ IC-002105

Pentabromooxomolybdate(*V*)(2−), 9CI
[17523-72-7]

$[MoOBr_5]^{2\ominus}$

M 511.4 (ion)
Di-H compd.: [25621-13-0].
Br_5H_2MoO M 513.4
Prepd. by HBr reduction of MoO_3. Reddish-brown cryst.
Di-NH_4 salt: [18253-22-0].
Prepd. by HBr reduction of $(NH_4)_2MoO_4$. Reddish-brown cryst. Sol. H_2O.

[36466-24-7, 36466-25-8, 86881-08-5]

Dalton, L.A. *et al*, *Inorg. Chem.*, 1969, **8**, 2477 (*esr*)
Saha, H.K. *et al*, *J. Indian Chem. Soc.*, 1969, **46**, 680 (*synth*)
Inorg. Synth., 1974, **15**, 100 (*synth*)
Fergusson, J.E. *et al*, *Inorg. Chim. Acta*, 1983, **71**, 29 (*synth, cryst struct*)

$Br_5NOOs^{2\ominus}$ IC-002106

Pentabromonitrosylosmate(2−)
[55031-52-2]

$[OsBr_5NO]^{2\ominus}$

M 619.7 (ion)
Synth. by heating $Na_2[OsNO(NO_2)_4OH]$ in HBr with subsequent treatment with MBr (M = NH_4, K, Rb, Cs, R_4N).
Di-K salt: [39554-00-2].
Opaque red-brown cryst.
Di-Rb salt: Brown-red powder. Spar. sol. H_2O. Dec. at 440°.
Di-NH_4 salt: [39609-01-3].
Brownish red cryst. (HBr). Dec. at 400°.

Sinitsyn, N.M. *et al*, *Koord. Khim.*, 1975, **1**, 103; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1975, **1**, 82.
Kravchenko, V.V. *et al*, *Koord. Khim.*, 1975, **1**, 930; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1975, **1**, 788 (*nqr*)
Bolshakov, K.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1979, **219**, 349 (*ir, uv*)
Nikolskii, A.B. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1980, **250**, 902 (*props*)
Sinitsyn, N.M. *et al*, *Zh. Neorg. Khim.*, 1980, **25**, 780 (*kinetics*)
Linko, I.V. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 1520 (*pe*)
Nefedov, V.I. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1986, **291**, 614 (*pe*)
Kravchenko, E.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1987, **294**, 130 (*nqr*)
Kravchenko, E.A. *et al*, *Koord. Khim.*, 1988, **14**, 49; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1988, **14**, 34 (*nqr*)
Salomov, A.S. *et al*, *Zh. Neorg. Khim.*, 1988, **33**, 2608 (*ir*)
Bobkova, E.Y. *et al*, *Zh. Neorg. Khim.*, 1990, **35**, 981 (*ir, raman*)
Svetlov, A.A. *et al*, *Zh. Neorg. Khim.*, 1990, **35**, 1767; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1990, **35**, 549 (*synth, props*)

$Br_5NORe^{2\ominus}$ IC-002107

Pentabromonitrosylrhenate(2−), 9CI
[44627-93-2]

$[Re(NO)Br_5]^{2\ominus}$

M 615.7 (ion)
Ir ν_{NO} 1715 cm^{-1}.
Di-Cs salt: [31332-83-9].
Synth. from Ag_2ReBr_6 and NO at 300° followed by EtOH extraction and treatment with HBr conc. and CsBr. Brown cryst.
Bis-Et_4N salt: [37549-21-6].

Synth. (i) from $Re(OEt)(PPh_3)_2Br_2$, NO and Me_4NBr in EtOH, (ii) from K_2ReBr_6, Et_4NBr, HBr and NO in EtOH. Pale green cryst. (EtOH). Mp 250° dec.

Giusto, D. *et al*, *Gazz. Chim. Ital.*, 1972, **102**, 265 (*synth, ir, props*)
Rakshit, S., *J. Inorg. Nucl. Chem.*, 1974, **36**, 2271 (*synth, ir, uv, props*)

$Br_5NORu^{2\ominus}$ IC-002108

Pentabromo(nitrosyl)ruthenate(2−), 9CI
[19592-08-6]

$[Ru(NO)Br_5]^{2\ominus}$ (C_{4v})

M 530.5 (ion)
Prepd. by treating $[Ru(NO)Cl_5]^{2\ominus}$ or $[Ru(NO)(OH)(NO_2)_4]^{2\ominus}$ with aq. HBr. Sol. H_2O.
Di-Na salt: [21058-81-1].
Br_5NNa_2ORu M 576.5
Raman ν_{RuBr_5} 179 cm^{-1} (H_2O).
Di-K salt: [14973-01-4].
Br_5K_2NORu M 608.7
Ir ν_{NO} 1881; ν_{RuBr_5} 260; ν_{RuBr} 176 cm^{-1}.
Di-Rb salt: [21058-82-2].
Br_5NORb_2Ru M 701.5
Ir ν_{NO} 1872; ν_{RuBr_5} 260 cm^{-1}.
Di-Cs salt: [16449-92-6].
Br_5Cs_2NORu M 796.4
Ir ν_{NO} 1840; ν_{RuBr_5} 252; ν_{RuBr} 173cm^{-1}.
Di-NH_4 salt: [13815-01-5].
$Br_5H_8N_3ORu$ M 566.6
Ir ν_{NO} 1870; ν_{RuBr_5} 255 cm^{-1}.
Bis-Me_4N salt: Ir ν_{NO} 1840; ν_{RuBr_5} 247 cm^{-1}.
Bis-Et_4N salt: Ir ν_{NO} 1832; ν_{RuBr_5} 245 cm^{-1}.

Gans, P. *et al*, *Inorg. Chem.*, 1966, **5**, 1877 (*ir*)
Durig, J.R. *et al*, *Spectrochim. Acta*, 1966, **22**, 1091 (*synth, ir*)
Sinitsyn, N.M. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1968, **9**, 36 (*ir*)
Miki, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1969, **42**, 3007 (*ir*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir*)
Veal, J.T. *et al*, *Inorg. Chem.*, 1972, **11**, 1420 (*synth*)
Cleare, M.J. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 2013 (*ir*)
Sinitsyn, N.M. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 1373 (*solv extraction*)
Nikol'skii, A.B. *et al*, *Zh. Fiz. Khim.*, 1977, **51**, 1822; *CA*, 1977, **87**, 126480 (*ir, ^{15}NO exchange*)

$Br_5NRu^{2\ominus}$ IC-002109

Pentabromonitridoruthenate(*VI*)(2−), 9CI
[53149-85-2]

$[N{\equiv}RuBr_5]^{2\ominus}$ (C_{4v})

M 514.5 (ion)
Di-Cs salt: [38882-97-2].
Br_5Cs_2NRu M 780.4
Prepd. by treating $[RuO_2Br_4]^{2\ominus}$ with $Na[N_3]$ in aqueous HBr, followed by CsBr. Brown, diamagnetic solid. Ir $\nu_{Ru{\equiv}N}$ 1046; ν_{RuBr} 204 cm^{-1}.

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1313 (*synth*)
Collin, R.J. *et al*, *J. Mol. Struct.*, 1973, **19**, 531 (*ir, raman*)

$Br_5NTc^{2\ominus}$ IC-002110

Pentabromonitridotechnetate(*VI*)(2−)

$[N{\equiv}TcBr_5]^{2\ominus}$ (C_{4v})

M 512.4 (ion)
Octahedral anion. Synth. from $TcO_4^{\ominus}$, $N_3^{\ominus}$, and conc. HBr. Dissociates completely to $[TcNBr_4]^{\ominus}$ + $Br^{\ominus}$ on dissolution.
Di-Cs salt: [110303-55-4].
Br_5Cs_2NTc M 778.2
Blue-black solid. Mp > 360°.

Baldas, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 1721 (*synth, ir, reactions*)

$Br_5N_3ReS_2^{2\ominus}$ IC-002111

Tetrabromo(monothiazyl monobromide-*N*)(thionitrosyl)rhenate(2−), 11CI

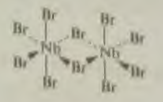
$[ReBr_4(NS)(NSBr)]^{2\ominus}$

M 677.8 (ion)
cis-form
Bis-Ph_4P salt: [105034-11-5].
Synth. from $ReBr_4(N_2S_2)^{\ominus}$ and PPh_4Br in CH_2Br_2. Red, needle-like cryst. +CH_2Br_2 (CH_2Br_2/hexane)

Hauck, H.G. *et al*, *Z. Anorg. Allg. Chem.*, 1986, **534**, 77.
Hauck, H.G. *et al*, *Z. Naturforsch., B*, 1986, **41**, 825 (*synth, ir, cryst struct*)

Br_5Nb IC-002112

Niobium(*V*) bromide ($NbBr_5$), 11CI
Niobium pentabromide
[13478-45-0]



dimer

M 492.4
Bioctahedral dimer in solid state, tbp monomer in gas phase. Synth. from Nb or Nb_2O_5 and Br_2 or from $NbCl_5$ and BBr_3. Yellow-red volatile solid. Mp 254-268°. Bp 365°. Readily hydrol. Forms solid solns. with $NbCl_5$.
Dimer: Di-μ-bromooctabromadiniobium(V)
$Br_{10}Nb_2$ M 984.8

Alexander, K.M. *et al*, *J. Chem. Soc.*, 1949, 3223 (*synth*)
Spitsbonov, V.P. *et al*, *Vestn. Mosk. Univ., Ser. 2: Khim.*, 1966, **21**, 109 (*pd*)
Dornseiner, R. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 3056 (*cryst struct, solid solns*)
Druce, P.M. *et al*, *J. Chem. Soc. A*, 1971, 1595 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1448 (*synth*)
Mueller, U. *et al*, *Z. Naturforsch., B*, 1983, **38**, 559 (*synth, cryst struct, β-form*)

$Br_5ORe^{2\ominus}$ IC-002113

Pentabromooxorhenate(*V*)(2−)
[30289-89-5]

$[O{=}ReBr_5]^{2\ominus}$ (C_{4v})

M 601.7 (ion)
Octahedral.
Di-Cs salt: [18222-40-7].
Synth. (i) as for Pentachlorooxorhenate(*V*)(2−), IC-017218, using HBr for HCl and CsBr for CsCl, (ii) by treatment of $ReOBr_3$ with 48% HBr followed by addition of CsBr. Cryst.

Edwards, D.A. *et al*, *J. Mol. Struct.*, 1970, **5**, 421 (*ir, ms, struct*)

Edwards, D.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 145 (*synth*)
Fergusson, J.E. *et al*, *Inorg. Chim. Acta*, 1983, **71**, 29 (*synth, struct*)

IC-002114

$Br_5ORe^{\ominus}$

Pentabromooxorhenate(*VI*)(1−), 9CI

[40782-74-9]

$[ReOBr_5]^{\ominus}$

M 601.7 (ion)
Ir $\nu_{Re=O}$ 950 cm^{-1}.
Ph_4P salt: [34852-91-0].
Synth. from $ReOBr_4$ and PPh_4Br in $CHCl_3$. Sol. $MeNO_2$.

Edwards, D.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 89 (*synth, ir, props*)

IC-002115

$Br_5OTc^{2\ominus}$

Pentabromooxotechnetate(*V*)(2−)

[95674-35-4]

$[O{=}TcBr_5]^{2\ominus}$ (C_{4v})

M 514.4 (ion)
Prone to dissociate into $TcOBr_4^{\ominus}$ + $Br^{\ominus}$.
Di-Cs salt: [86881-09-6].
Br_5Cs_2OTc M 780.2

Hanuza, J. *et al*, *Acta Phys. Pol. A*, 1987, **71**, 91 (*ir*)
Hanuza, J. *et al*, *J. Mol. Struct.*, 1987, **158**, 43 (*ir*)

IC-002116

$Br_5OU^{2\ominus}$

Pentabromooxouranate(*V*)(2−)

$[UOBr_5]^{2\ominus}$

M 653.5 (ion)
Bis-Et_4N salt: [30917-62-5].
Green solid + 2.5 Et_4NBr. Ir $\nu_{U=O}$ 919, 817 cm^{-1}.
Bis-Ph_4As salt: [30917-61-4].
Green solid.

Ryan, J.L., *J. Inorg. Nucl. Chem.*, 1971, **33**, 153 (*synth, ir, uv-vis*)
Selbin, J. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 3467.
Selbin, J. *et al*, *Inorg. Chem.*, 1974, **13**, 1235 (*synth, esr*)

IC-002117

$Br_5OW^{2\ominus}$

Pentabromooxotungstate(*V*)(2−), 9CI

[36695-46-2]

$[WOBr_5]^{2\ominus}$

M 599.3 (ion)
Prepd. from $[WO_2(C_2O_4)_2]^{3\ominus}$ and aq. HBr.
Di-Rb salt:
Br_5ORb_2W M 770.3
Yellow-brown cryst.
Di-Cs salt: [18131-75-4].
Br_5Cs_2OW M 865.1
Greenish-yellow powder.

Paulssen v Beck, H., *Z. Anorg. Allg. Chem.*, 1931, **196**, 85 (*synth*)
Allen, E.A. *et al*, *J. Chem. Soc.*, 1963, 4649 (*synth, uv*)
Brisden, B.J. *et al*, *J. Chem. Soc. A*, 1967, 1825 (*uv, magnetism*)

Br_5P

Phosphorus bromide (PBr_5), 8CI IC-002118

Pentabromophosphorane, *9CI. Phosphorus pentabromide. Pentabromophosphorus*(V). *Tetrabromophosphonium bromide*

[7789-69-7]

$[PBr_4^{\oplus}]Br^{\ominus}$

M 430.4
Orthorhombic. $P^{\oplus}$—Br 215 pm. Ordered lattice at r.t. Quenching (to 15K) and warming to 18K gives disordered lattice of same composition. Synth. by reaction of P or PBr_3 + Br_2. Commercially available brominating agent. Reddish yellow rhombohedral cryst. ($PhNO_2$) at r.t. Dec. at b.p. with dissoc. of vapour into PBr_3 + Br_2. Bp 106° dec. ΔH_f° −46 kJ mol^{-1}.
▷ Corrosive, poison. TH3980000.
Br_2 adduct (1:1): see *Tetrabromophosphonium tribromide, IC-002205*

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 499 (*rev, bibl*)
Wieker, W. *et al*, *Z. Naturforsch., B*, 1966, **21**, 1103 (*P-31 nmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 865 (*use*)
Gabes, W. *et al*, *Acta Crystallogr., Sect. B*, 1970, **26**, 443 (*cryst struct*)
Dhamelincourt, P. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 2470 (*raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 522, 1147 (*rev*)
Gabes, W. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1971, **90**, 157 (*raman*)
Kravchenko, E.A. *et al*, *Zh. Neorg. Khim.*, 1975, **20**, 2556; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 1416 (*nqr*)
Finch, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1981, 812 (*raman, struct*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2778.

IC-002119

Br_5Pa

Protactinium(*V*) bromide ($PaBr_5$)

Protactinium pentabromide

[15608-38-5]

$PaBr_5$

M 630.5
Synth. from PaC + Br_2 (350°); or from Pa_2O_5 + C + Br_2 (600-700°). V. moisture-sensitive red or orange-brown cryst. Sol. MeCN. Subl. 300° *in vacuo*, Bp 428° (extrap.).

α-form

β-form

Possesses the α-UCl_5 struct. with six-coordinate Pa.

γ-form

Isostructural with β-UCl_5.

Asprey, L.B. *et al*, *Inorg. Chem.*, 1966, **6**, 659 (*synth*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1966, 262; 1970, 476; 1976, 1336 (*synth, ir*)
Brown, D. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 178 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1177 (*synth*)
Brown, D. *et al*, *Inorg. Nucl. Chem. Lett.*, 1979, **15**, 219 (*cryst struct*)

IC-002120

$Br_5Pb_2^{\ominus}$

μ-Bromotetrabromodiplumbate(1−), 9CI

Pentabromodiplumbate(1−)

$[Pb_2Br_5]^{\ominus}$

M 813.9 (ion)
Occurs as a variety of salts having mainly tetragonal or orthorhombic structs.
Rb salt: [12380-89-1]. *Lead rubidium bromide. Dilead rubidium pentabromide*
Br_5Pb_2Rb M 899.3
Synth. from $PbBr_2$ and RbBr in H_2O. Tetragonal cryst.
ΔH_f −56.43 kJ mol^{-1}.
NH_4 salt: [12628-16-9]. *Ammonium lead bromide ($(NH_4)Pb_2Br_5$)*
Synth. from $[NH_4]Br$ + $PbBr_2$ in H_2O. Orthorhombic cryst.

Jansen, P.W.J., *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1968, **87**, 1021 (*cryst struct, synth, derivs*)
Cola, M. *et al*, *Z. Naturforsch., A*, 1971, **26**, 1328 (*phase diagram, struct, Rb salt*)

IC-002121

Br_5Re

Rhenium(*V*) bromide ($ReBr_5$)

Rhenium pentabromide

[30937-53-2]

$ReBr_5$

M 585.7
Not fully characterised. Synth. from $ReBr_3$ and Br_2 at 170-240°.

Colton, R., *J. Chem. Soc.*, 1962, 2078.
Ovchinnikov, K.V. *et al*, *Zh. Obshch. Khim.*, 1972, **42**, 1180, 1183 (*synth, thermodynamic props*)

IC-002122

Br_5Sb

Antimony(*V*) bromide ($SbBr_5$), 9CI, 8CI

Pentabromoantimony(V). *Antimony pentabromide*

[29702-86-1]

$SbBr_5$

M 521.2
Evidently unknown in the free state. An etherate has been reported, and complexes derived from $SbBr_5$ are also known.

Et_2O complex: Pentabromo(diethyl ether)antimony
$C_4H_{10}Br_5OSb$ M 595.3
Solid. Loses Et_2O and Br_2 at sl. above r.t.

Holmes, R.R., *J. Inorg. Nucl. Chem.*, 1961, **19**, 363 (*attempted synth*)
Adams, C.J. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 1829 (*complexes*)

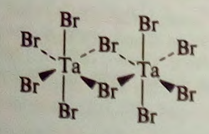
IC-002123

Br_5Ta

Tantalum(*V*) bromide ($TaBr_5$), 11CI

Tantalum pentabromide

[13451-11-1]



dimer

M 580.4
Bioctahedral dimer in solid state, tbp monomer in gas phase. Synth. from Ta, Ta_2O_5 or $TaCl_5$ and various brominating agents. Volatile yellow-red solid. Mp 256-280°. Bp 344-348°. Readily hydrol.
Dimer: Di-μ-bromooctabromoditantalum(V)

$Br_{10}Ta_2$ M 1160.9

Skinner, H.A. *et al*, *Trans. Faraday Soc.*, 1940, **36**, 668 (*ed*)
Canterford, J.H. *et al*, *Halides of the Second and Third Row Transition Metals*, Wiley, N.Y., 1968, 158 (*synth, props*)
Merlin, J.C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1971, **272**, 53 (*raman*)
Druce, P.M. *et al*, *J. Chem. Soc. A*, 1971, 3595 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1455 (*synth*)

IC-002124

$Br_5Tl^{2\ominus}$

Pentabromothallate(*III*)(2−)

$[TlBr_5]^{2\ominus}$

M 603.9 (ion)
Solid does not contain discrete $[TlBr_5]^{2\ominus}$ units.
▷ Toxic.
Di-Cs salt:
Br_5Cs_2Tl M 869.7
Synth. from aq. $TlBr_3$/CsBr mixt. Cryst; dec. to $Cs_3Tl_2Br_9$/CsBr at 260°. Struct. related to Scheelite with both tetrahedral $[TlBr_4]^{\ominus}$ and octahedral $[TlBr_6]^{3\ominus}$ units.

Zimmermann, K. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **553**, 280.

IC-002125

$Br_5U^{2\ominus}$

Pentabromouranate(*III*)(2−)

$UBr_5^{2\ominus}$

M 637.5 (ion)
Di-K salt: [53513-84-1].
Br_5K_2U M 715.7
Dark violet solid. Mp 580°. 6-Coord., isotypic with Cs_2DyCl_5. Ir ν_{U-Br} 145, 124, 110 cm^{-1}.
Di-Rb salt: [53513-86-3].
Br_5Rb_2U M 808.4
Dark violet solid. Mp 532° dec. 6-Coord., isotypic with Cs_2DyCl_5. Ir ν_{U-Br} 144, 124, 111 cm^{-1}.
Di-Cs salt: [53513-88-5].
Br_5Cs_2U M 903.3
Dark violet solid. Mp 420° dec. 6-Coord., isotypic with Cs_2DyCl_5. Ir ν_{U-Br} 140, 124, 110 cm^{-1}.

Vdovenko, V.M. *et al*, *Radiokhimiya*, 1974, **16**, 369; *Sov. Radiochem. (Engl. Transl.)*, 1974, **16**, 369 (*synth*)
Suglobova, I.G. *et al*, *Radiokhimiya*, 1978, **20**, 352, 365; *Sov. Radiochem. (Engl. Transl.)*, 1978, **20**, 302, 310 (*struct, ir*)
Suglobova, I.G. *et al*, *Koord. Khim.*, 1981, **7**, 97; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1981, **7**, 53 (*synth*)
Volkov, V.A. *et al*, *Radiokhimiya*, 1987, **29**, 273; *Sov. Radiochem. (Engl. Transl.)*, 1987, **29**, 259 (*struct*)

IC-002126

Br_5U

Uranium(*V*) bromide (UBr_5)

Uranium pentabromide

[13775-16-1]

UBr_5

M 637.5
Possesses the β-UCl_5 struct. Synth. from U + Br_2 at 80° or from UBr_4 + Br_2. Dark reddish-brown solid. Sol. EtOH, Me_2CO, EtOAc.

Prigent, J., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1954, **238**, 102 (*synth*)
Lux, F. *et al*, *Chem. Ber.*, 1970, **103**, 2807 (*synth*)
Blair, A. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 3795 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1213 (*synth*)

Lery, J.H. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1055 (*cryst struct*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1385 (*synth*)
Bohrer, R. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **558**, 119 (*synth*)

IC-002127

Br_5W
Tungsten bromide (WBr_6)
Tungsten pentabromide
[13470-11-6]

WBr_5

M 583.3
Prepd. from W + Br_2 at 650°. Hygroscopic dark-brown needles. Hydrol. by water. Mp 276°. Bp 333°.

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1931, **11**, 853.
Brown, T.M. *et al*, *Inorg. Chem.*, 1967, **6**, 1335 (*synth*)

IC-002128

$Br_5Zn^{3\ominus}$
Pentabromozincate(3−)
$[ZnBr_5]^{3\ominus}$

M 464.9 (ion)
Salts probably all contain anions $[ZnBr_4]^{2\ominus}$ and $Br^{\ominus}$.
Tri-Rb salt: [38257-07-7].
Br_5Rb_3Zn M 721.3
Air-stable white cryst. Compd. consists of $Rb^{\oplus}$, $Br^{\ominus}$ and $[ZnBr_4]^{2\ominus}$ ions. Isomorphouswith $(NH_4)_3ZnCl_5$.
Cs salt: [59273-13-1].
Br_5Cs_3Zn M 863.6
Cryst.
Tri-NH_4 salt: [38257-08-8].
Cryst.
[59273-13-1]

Asker, W.J. *et al*, *Austr. J. Chem.*, 1972, **25**, 2301 (*synth, nqr*)
Hennig, M. *et al*, *Z. Naturforsch., A*, 1981, **36**, 286 (*cryst struct, Rb salt*)
Pirnat, J. *et al*, *Phys. Status Solidi A*, 1982, **74**, K55 (*nqr, Rb salt*)

IC-002129

$Br_5Zn_2^{\ominus}$
μ-Bromotetrabromodizincate(1−)
$[Br_3Zn{-}Br{-}ZnBr_3]^{\ominus}$

M 530.3 (ion)
Cs salt: [117504-89-9]. *Caesium zinc bromide ($CsZn_2Br_5$)*
$Br_5Cs_1Zn_2$ M 663.2
Cryst. Mp 225°. Two polymorph. forms, transition at 215°.

Kuznetsova, I.Ya. et al, Russ. J. Inorg. Chem. (Engl. Transl.), 1988, 33, 1202 (phase diagram, $ZnBr_2/CsBr$ powder struct)

IC-002130

$Br_6C4^{4\ominus}$
Hexabromocadmiate(4−)
[65338-12-7]

$[CdBr_6]^{4\ominus}$

M 591.8 (ion)
Formed from $CdBr_2$ + AsBr in AcOH soln.
[7789-70-0, 10326-41-2, 12318-97-9]

Goubeau, M. et al, CA, 1967, 66, 69833a (synth, cryst struct)
Hieth, H.G. et al, Z. Anorg. Allg. Chem., 1971, 380, 56 (synth)

IC-002131

$Br_6Ce^{2\ominus}$
Hexabromocerate(*IV*)(2−)
$[CeBr_6]^{2\ominus}$

M 619.5 (ion)
Bis-Et_4N salt: [17116-11-9].
Moisture-sensitive deep violet solid.
Bis-Ph_3PH salt: [54595-33-4].
Moisture-sensitive deep violet solid.

Ryan, J.L. *et al*, *J. Phys. Chem.*, 1966, **70**, 2845 (*synth*)
Ryan, J.L., *Inorg. Chem.*, 1969, **8**, 2053 (*synth*)
Inorg. Synth., 1974, **15**, 231 (*synth*)

IC-002132

$Br_6Cl^{\ominus}$
Hexabromochlorate
Chlorohexabromate

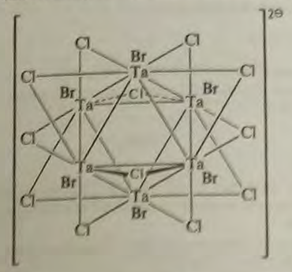
Struct. unknown

M 514.8 (ion)
Et_4N salt: Synth. from $[Et_4N]Cl$ and Br_2 in a desiccator. Dark red cryst. powder. Mp 53°. Exists at r.t. only under Br_2.

Chattaway, F.D., *J. Chem. Soc.*, 1923, **123**, 654 (*synth*)

IC-002133

$Br_6Cl_{12}Ta_6^{2\ominus}$
Hexabromododeca-μ-chlorohexatantalate(2−), 11Cl



M 1990.5 (ion)
Bis-Et_4N salt: [12555-91-8].
Synth. by oxidising $[Ta_6Cl_{12}]^{2\oplus}$ in EtOH with Br_2, adding $[Et_4N]Br$ and saturating with HBr. Red solid (EtOH).
Bis-tetrabutylammonium salt: [68758-52-1].
Synth. by saturating a soln. of $[Ta_6Cl_{12}]Cl_2{\cdot}8H_2O$ in EtOH with HBr, adding $[Bu_4N]Br$ and further HBr. Dark red solid.
Bis-pyridinium salt: [11127-28-9].
Red solid.

Spreckelmeyer, B., *Z. Anorg. Allg. Chem.*, 1969, **368**, 18 (*synth*)
Hughes, B.G. *et al*, *Inorg. Chem.*, 1970, **9**, 1343 (*synth*)
Fleming, P.B. *et al*, *Inorg. Chem.*, 1970, **9**, 1769 (*ir*)
Best, S.A. *et al*, *Inorg. Chem.*, 1979, **18**, 684 (*synth, pe*)

IC-002134

$Br_6Cr^{4\ominus}$
Hexabromochromate(*II*)(4−), 9Cl

$[CrBr_6]^{4\ominus}$

M 531.4 (ion)
Bis-piperazinedium salt: [77152-47-7].
Light green.
Bis-piperazinedium salt dihydrate: [77152-48-8].

Prepd. from $CrBr_2{\cdot}H_2O$ and piperazine.2HBr in HBr. Light blue cryst.

Babar, M.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 27 (*synth, uv, magnetism*)

IC-002135

$Br_6Cr^{3\ominus}$
Hexabromochromate(*III*)(3−)
[36830-79-2]

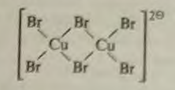
$[CrBr_6]^{3\ominus}$

M 531.4 (ion)
Di-Cs, mono-Li salt: [69275-98-5].
Br_6CrCs_2Li M 804.1
Prepd. from CsBr, Li_2CO_3 and Cr_2O_3 in HBr solns.

Meyer, G. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1476 (*synth, cryst struct*)

IC-002136

$Br_6Cu_2^{2\ominus}$
Di-μ-bromotetrabromodicuprate(*II*)(2−), 8Cl
Hexabromodicuprate(2−). Tribromocuprate(1−) dimer

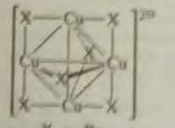


M 606.5 (ion)
Antiferromagnetically coupled dimer.
Di-K salt: [17568-01-3].
$Br_6Cu_2K_2$ M 684.7
Dark-brown needle-like cryst.
Di-Cs salt:
$Br_6Cs_2Cu_2$ M 872.3
Dark-brown prismatic cryst.
Di-NH_4 salt: [77489-89-5].
Bis-Ph_4As salt: [52873-77-5].

Inoue, M. *et al*, *Inorg. Chem.*, 1967, **6**, 900 (*synth, magnetism*)
Willett, R.D. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 2482 (*uv*)
Chow, C. *et al*, *Inorg. Chem.*, 1975, **14**, 205 (*magnetism*)
O'Bannon, G. *et al*, *Inorg. Chim. Acta*, 1981, **53**, L131 (*magnetism*)

IC-002137

$Br_6Cu_4^{2\ominus}$
Hexa-μ-bromo-*tetrahedro*-tetracuprate(2−)



X = Br

M 733.6 (ion)
Tetrahedron of Cu atoms within octahedron of bromide ligands. Cu—Cu distances 271.8-275.0 pm.
Bis-tetrapropylammonium salt: [94118-31-7].
Cryst. (EtOH).
Bis-butyltriphenylphosphonium salt: [105011-13-0].
Colourless octahedra (EtOH). Mp 123-124°.

Asplund, M. *et al*, *Acta Chem. Scand., Ser. A*, 1984, **38**, 725 (*synth, cryst struct*)
Andersson, S. *et al*, *Acta Chem. Scand., Ser. A*, 1986, **40**, 210 (*cryst struct, $BuPh_3P$ salt*)

IC-002138

$Br_6Eu^{3\ominus}$
Hexabromoeuropate(*III*)(3−)
[52637-58-8]

$[EuBr_6]^{3\ominus}$ (O_h)

M 631.3 (ion)
Di-Cs, Na salt: [69207-90-5].
Br_6Cs_2EuNa M 920.1
Yellow cryst. Possesses elpasolite struct.
Tris-pyridinium salt: [31869-50-8].
Cryst. ν_1 156, ν_5 164 cm^{-1}.
Tris-Ph_3PH salt: Deliquescent orange-yellow cryst. + $1Ph_3PHBr$. ν_1 155, ν_5 164 cm^{-1}.

Ryan, M. *et al*, *J. Phys. Chem.*, 1966, **70**, 2845 (*synth, uv-vis*)
Choca, M. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 1425 (*synth, ir, raman*)
Meyer, G. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1476 (*synth, struct*)

IC-002139

$Br_6GaIn^{2\ominus}$
Tribromo(tribromogallate)indate(2−), 10Cl
Hexabromogallateindate(2−)

$[Br_3Ga{-}InBr_3]^{2\ominus}$

M 663.9 (ion)
Bis-tetrabutylammonium salt: [81182-74-3].
Synth. from Gallium indium bromide ($GaInBr_6$), IC-002018 and $[Bu_4N]Br$. White moisture-sensitive solid.

Sinclair, I. *et al*, *Inorg. Nucl. Chem. Lett.*, 1981, **17**, 279 (*synth, raman*)

IC-002140

$Br_6Ga_2^{2\ominus}$
Hexabromodigallate(2−)
[25395-73-7]

$[Br_2Ga{-}GaBr_2]^{2\ominus}$ (D_{3d})

M 618.8 (ion)
Raman ν_{Ga-Ga} 164 cm^{-1}.
Di-Ga(1) salt: [53817-19-7]. *Gallium bromide ($GaBr_{1.5}$)*
Br_6Ga_4 M 758.3
Synth. from $GaBr_3$ and Ga at 180°. White solid.
Bis-Me_4N salt: [41618-77-5].
Synth. by anodic oxidation of Ga in 6M HBr and precipitation with $[Me_4N]Br$. Colourless cryst. (Me_4NO_3). Spar. sol. EtOH. Other R_4N salts also exist.
Bis-Ph_3PH salt: [77187-71-6].
Colourless cryst. Mp 166-162°.
Bis-Ph_4P salt: Colourless cryst. (Me_2NO_3). Sol. Me_2NO_3. Mp 215°.

Evans, C.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 988 (*synth, ir, raman*)
Wilkinson, M. *et al*, *Inorg. Nucl. Chem. Lett.*, 1974, **10**, 747 (*synth, $GaBr_{1.5}$*)
Klaui, M. *et al*, *Inorg. Nucl. Chem. Lett.*, 1980, **16**, 469 (*synth*)
Inorg. Synth., 1983, **22**, 110 (*synth*)

IC-002141

Br_6HSb
Hydrogen hexabromoantimonate(*V*)(1−), 9Cl, 8Cl

$H[SbBr_6]$

M 602.1
Known derivs. have struct. more complex than molecular formula suggests.
Trihydrate: [117565-24-9].

Structure contains octahedral $TcBr_6^{2-}$ ions and water-bridged dimers of $(H_2O)_5Tc(\mu\text{-}OH_2)Tc(OH_2)_5$. Synth. from $TcBr_3$, Br_2 + HBr aq. Reactive, irregular hexagonal deliquescent black plates. Mp dec. 120°.

Pt- salt: see Hexahydrogen

tetrakis(carbonato-tetraoxomanganate(III,V)) IC-002/300

Gmelin Handbook Inorg. Chem., Syst. No. 10, 1940, 483 (rev.)

Hieber, H. et al. Z. Anorganikgr., 1967, **101**, 113 (synth, crystal struct)

IC-002142

Br_6H_2Tc

Hexabromotechnetic acid

Dihydrogen hexabromotechnetate(2−), 2HCl

[115435-07-9]

H_2TcBr_6

M 580.5

By-product of technetium-bromide cluster synth.

Diacetate: [118435-08-6]. *Bis-hydronium hexabromotechnetate. Diammonium hexabromotechnetate* Red crystal. Mod. sol. HBr, polar org. solvs. Distorted K_2PtCl_6 struct.

Kryuchkov, S.V. *et al. Zh. Neorg. Khim.*, 1987, **32**, 2933; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1987, **32**, 1714 (*synth, cryst struct, ir, pmr*)

IC-002143

Br_6H_2Te

Hexabromotelluric acid

H_2TeBr_6

M 609.0

Free acid H_2TeBr_6 unknown.

Di-NH_4 salt: Ammonium hexabromotellurate(IV)

(Diammonium hexabromotellurate(2−))

$Br_6H_8N_2Te$ M 643.1

From TeO_2 + NH_4Br in hot conc. aq. HBr. Bright red cryst. O_h geometry around Te. Interatomic distance Te—Br 270 pm.

Das, A.K. *et al. Can. J. Chem.*, 1966, **44**, 939 (*deriv. synth, cryst struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 11, 1978, **B3**, 40 (*bibl*)

IC-002144

Br_3H_3Sb

Trihydrogen hexabromoantimonate(*III*)(3−), 9Cl, 8Cl

Hexabromoantimonic(III) acid

$H_3[SbBr_6]$

M 604.1

Salts synth. from $SbBr_3$ + HBr aq. + amine

Tris-$EtNH_2$ salt: Solid. Mp 218°.

Tris-Et_2NH salt: [38333-00-5].

Pale yellow cryst. Mp 161°. Hexagonal.

Tris-diprop ylamine salt: Mp 128-130°. Monoclinic.

Tris-tripropylamine salt: [38333-05-0].

Solid. Mp 180°.

Tris-butylamine salt: [38415-23-5].

Cryst. Mp 194-196°. Orthorhombic.

Tris-aniline salt: [59450-18-9].

Solid. Mp 188°

Gmelin Handbook Inorg. Chem., Syst. No. 18, 1949, 482 (*rev, bibl*)

Jha, N.K. *et al. J. Inorg. Nucl. Chem.*, 1972, **34**, 2953; 1976, **38**, 401 (*synth*)

Hoisger, H.A. *et al, Aust. J. Chem.*, 1973, **26**, 1401 (*synth, ir, raman*)

Kolditz, L. *et al, Z. Anorg. Allg. Chem.*, 1973, **395**, 227 (*uv*)

Jha, N.K. *et al. J. Inorg. Nucl. Chem.*, 1976, **38**, 1479 (*synth, prepr, cryst struct*)

Lewis, J.F. *et al, Bull. Soc. Chim. Fr.*, 1979, 120 (*synth, raman*)

Okuda, T. *et al, Chem. Lett.*, 1982, 1321 (*prepr, cryst struct*)

Okuda, T. *et al, Z. Naturforsch., A*, 1986, **41**, 319 (*prepr*)

IC-002145

$Br_6H_4Mo_2O_2^{2-}$

Diaquahexabromodimolybdate(*II*)(2−), HCl, 10Cl, 9Cl

Bis(tribromodiaquadimolybdate(II)(2−))

M 707.3 (ion)

Eclipsed config. about quadruple Mo—Mo bond; interatomic distance Mo—Mo 213.0 pm. Isostructural with Diaquahexachlorodimolybdate(*II*)(2−), IC-01727.

Bis-pyridinium salt: [68780-18-7].

Synth. from $(NH_4)_4Mo_2Cl_8H_2O$ + [PyH]Br in aq. HBr. Cryst. (aq. HBr/[PyH]Br). Sol. H_2O dec. Formulated as $(PyH)_2[Mo_2Br_6(OH_2)_2]Br$.

Bis-4-methylpyridinium salt: [59949-43-8].

Cryst. Stable in dry air. Sol. H_2O; sl. sol. MeOH, MeCN. Diamagnetic.

Bis-morpholinium salt: [81445-62-7].

Synth. from $[NH_4]_4Mo_2Cl_8H_2O$ in HBr and morphinium hydrobromide at 0°. Cryst. + HBr. Dec. at 87°

Bis-piperidium salt: [73745-07-0].

Brencic, J.V. *et al, Z. Anorg. Allg. Chem.*, 1976, **423**, 266; 1978, **444**, 211 (*cryst struct, synth*)

Brencic, J.V. *et al, Vestn. Slov. Kem. Drus.*, 1979, **26**, 367 (*cryst struct*)

Brencic, J.V. *et al, Inorg. Chim. Acta*, 1982, **57**, 247 (*cryst struct, synth*)

IC-002146

$Br_6H_8N_2Sb$

Diammonium hexabromoantimonate(2−), 9Cl, 8Cl

[30660-75-4]

$[NH_4]_4[Sb^{III}Br_6][Sb^{V}Br_6]$ (dimer)

M 637.2

Dimeric-form

$Br_{12}H_{16}N_4Sb_2$ M 1274.5

Tetragonal. Anions arranged in ordered array with like Sb-oxidation states repeating along *a* and *b* directions, but alternating along *c* axis. The Sb(*III*) anions are undistorted but the Sb(*V*) ions are distorted. Interatomic distances: Sb^{III}—Br 279.5, Sb^{V}—Br 256.4 pm. Synth. from $SbBr_3$ + NH_4Br + Br_2 in HBr aq. Jet black cryst. (48% HBr aq.). Diamagnetic. Slowly and reversibly debrominated at r.t. to give yellow solid.

Lawton, S.L. *et al, Inorg. Chem.*, 1966, **5**, 743 (*synth, cryst struct*)

Adams, C.J. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 1829 (*synth, ir, raman*)

Clark, R.J.H. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1145 (*raman*)

Terao, H. *et al, Chem. Lett.*, 1981, 209 (*nqr*)

IC-002147

$Br_6H_8N_2Tc$

Diammonium hexabromotechnetate(*IV*) ($(NH_4)_2TcBr_6$)

[29462-54-2]

$(NH_4)_2TcBr_6$

M 614.4

Thermolysis gives Tc_4N_5.

[74493-13-9]

Vinogradov, I.V. *et al, Zh. Neorg. Khim.*, 1978, **23**, 1138; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 639 (*thermal*)

Chistalitov, V.N. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1982, **268**, 148 (*pct*)

Thompson, M. *et al, Anal. Chem.*, 1985, **58**, 3100 (*pct*)

IC-002148

$Br_6Hf^{2\ominus}$

Hexabromohafnate(*IV*)(2−), HCl

[33751-30-3]

$[HfBr_6]^{2\ominus}$

M 657.9 (ion)

Octahedral. Synth. by melting $HfBr_4$ and $2MBr_x$ in an evacuated silica tube. ΔH_f° −1793 kJ mol^{-1}.

Di-K salt: [91631-06-0]. *Potassium hexabromohafnate(IV)*

Br_6HfK_2 M 736.1

White solid.

Di-Cs salt: [66169-92-4]. *Caesium hexabromohafnate(IV)*

White solid. Proposed as a phosphor.

Bis-Et_4N salt: [21868-89-5].

Synth. by electrochemical oxidation of Hf in Br_2/THF soln. followed by addn. of Et_4NBr. Also by reaction of $HfBr_4$ and Et_4NBr in $SOBr_2$. White solid.

van Bronswyk, W. *et al, Inorg. Chem.*, 1969, **8**, 1395 (*synth, ir, raman*)

Haiseb, J.J. *et al, Can. J. Chem.*, 1977, **55**, 3882 (*electrochem synth*)

Makhiya, R. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1707 (*synth, thermochem, Cs salt*)

U.S. Pat., 4 496 844, (1985); *CA*, **102**, 176650 (*use*)

IC-002149

$Br_6Hg^{4\ominus}$

Hexabromomercurate(4−)

$[HgBr_6]^{4\ominus}$ (O_h)

M 680.0 (ion)

Tetra-Tl(I) salt: [51162-04-0]. *Thallium(I) hexabromomercurate (Tl_4HgBr_6). Mercury thallium(I) bromide ($HgTl_4Br_6$)*

Br_6HgTl_4 M 1497.5

Obt. from TlBr and $HgBr_2$. Cryst. Struct. contains isolated compressed $HgBr_6$ octahedra with Tl atoms between them.

Tetra-NH_4 salt: Cryst. Mp 266°.

Belyaev, I.M. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1950, **73**, 1217 (*synth, NH_4 salt*)

Huart, J., *Bull. Soc. Fr. Minéral. Cristallogr.*, 1965, **88**, 699; 1966, **89**, 23 (*thermal anal*)

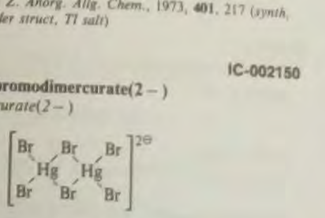
Brodersen, K. *et al, Z. Anorg. Allg. Chem.*, 1973, **401**, 217 (*synth, cryst struct, powder struct, Tl salt*)

IC-002150

$Br_6Hg_2^{2\ominus}$

Di-μ-bromotetrabromodimercurate(2−)

Hexabromodimercurate(2−)



M 880.6 (ion)

Hexaaquamagnesium(2+) salt:

$Br_6H_{12}Hg_2MgO_4$ M 1013.0

Yellow-gold needles. Mp 221° (closed tube), Mp 113° dec. (open tube).

Bis[[N,N-bis(2-aminoethyl)-1,2-ethanediamine-N,N',N'',N''']bromomercury(1+)] salt: [52654-51-0].

Cryst. (MeOH/2-propanol).

Di-M compd., tetrakis(triphenylarsine oxide) complex:

Synth. from Pb_3AsO_3HBr and $HgBr_2$. White cryst. Mp 146-147°. Ionic compd. made up of $[(Pb_3AsO_3)_4H]^{\oplus}$ cations and $[Hg_2Br_6]^{2\ominus}$ anions.

Bis-Et_4N salt: [61037-50-0].

Cryst.

Bis-tetrabutylammonium salt: [82861-65-2].

Cryst. Mp 100-102°.

Tris(tetrathiotetracene)(2+) salt: [85715-85-1]. *Salt with naphthacene(5,6-c,d:11,12-c',d')bis[1,2]dithiole (1:1)*

Cryst. Formulated as $[(TTT)_3]^{2\oplus}[Hg_2Br_6]^{2\ominus}$. Cation-radical chains stacked parallel to *c*-axis.

Tris(tetraselenotetracene)(2+) salt: [85715-87-3]. *Salt with naphthacene(5,6-c,d:11,12-c',d')bis[1,2]diselenole (1:1)*

Cryst. Formulated as $[(TSeT)_3]^{2\oplus}[Hg_2Br_6]^{2\ominus}$. Cation-radical chains stacked parallel to *c*-axis.

Harris, G.S. *et al, J. Chem. Soc., Chem. Commun.*, 1967, 442 (*synth, ir, conduct, cryst struct, $(Pb_3AsO_3)_4H$ salt*)

Ciampolini, M. *et al, Inorg. Chim. Acta*, 1973, **7**, 549 (*synth, conduct, ir, Br(tren)Hg salt*)

Barr, R.M. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1593 (*synth, ir, raman, Et_4N salt*)

Gal, A.W. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1976, **95**, 137 (*synth, ir, cryst struct, esr*)

Nelson, S.M. *et al, J. Chem. Soc., Chem. Commun.*, 1977, 167 (*synth, ir, uv, conduct, cryst struct, Hg macrocycle salt*)

Drew, M.G.B. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 375 (*ir, raman, Bu_4N salt*)

Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 875 (*synth, ir, raman, Bu_4N salt*)

Huira, M., *J. Sci. Hiroshima Univ. Ser. A: Phys. Chem.*, 1982, **45**, 383 (*Br-81 nqr, Et_4N salt*)

Shibaeva, R.P. *et al, Kristallografiya*, 1983, **28**, 296 (*cryst struct, tetracene salts*)

Brodersen, K. *et al, Z. Anorg. Allg. Chem.*, 1983, **502**, 209 (*synth, cryst struct, $[Mg(OH_2)_6]$ salt*)

IC-002151

$Br_6In^{3\ominus}$

Hexabromoindate(3−)

$[InBr_6]^{3\ominus}$ (O_h)

M 594.2 (ion)

Tri-Li salt: [41333-37-3]. *Lithium hexabromoindate (Li_3InBr_6)*

Br_6InLi_3 M 615.0

Synth. from LiBr—$InBr_3$ melt. White moisture sensitive solid. Mp 237°

Tri-Na salt: [33248-58-7].

Br_6InNa_3 M 663.2

Synth. from NaBr—$InBr_3$ melt. White moisture sensitive solid.

Tri-K salt: [41333-38-4].

Br_6InK_3 M 711.5

Synth. from KBr—$InBr_3$ melt. White moisture sensitive solid. Mp 320°

Tri-Rb salt: [72860-03-8].

Br_6InRb_3 M 850.6

White moisture sensitive solid.

Tri-Cs salt: [73556-95-3].

Br_6Cs_3In M 992.9

Synth. from CsBr, In_2O_3 and aq. HBr or from CsBr—$InBr_3$ melt. White moisture sensitive solid. Cs_2Li and Cs_2Na salts also descr.

Walter, P.H.L., *J. Inorg. Nucl. Chem.*, 1961, **19**, 223 (*phase diagram*)

Dudareva, A.G. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 1378; 1973, **18**, 109; 1974, **19**, 435 (*phase diagram*)

Davies, J.E. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 905 (*raman*)

Bogatov, Yu.E. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 517 (*ir*)
Meyer, G. *et al., Z. Naturforsch., B*, 1978, **33**, 1476 (*synth, cryst struct*)

IC-002152

$Br_6In_2^{2\ominus}$
Hexabromodiindate(2−)
$[Br_3In\text{-}InBr_3]^{2\ominus}$

M 709.0 (ion)
An 'ethane-like' anion.
Bis-tetrabutylammonium salt: [59643-24-2].
Synth. from In_2Br_4 + $[Bu_4N]Br$ in xylene. White powder. Spar. sol. Et_2O.
N,N'-Dimethyl-4,4'-bipyridinium(2+) salt: [59643-28-6].
(N,N'-Dimethyl-4,4'-bipyridinium) tetrabromoindate(1−) dibromoindate(1−)
Synth. from $[MebipyH_2][InBr_4]$ + $InBr_3$ in EtOH. Colourless solid. Spar. sol. MeOH, sol. MeCN. Shown to be $[Me_2bipyH_2][InBr_4][InBr_2]$.

Davies, J.E. *et al., J. Inorg. Nucl. Chem.*, 1974, **36**, 805 (*raman*)
Freeland, B.H. *et al., Inorg. Chem.*, 1976, **15**, 2144 (*synth, ir, raman*)
McGarvey, B.R. *et al., Inorg. Chem.*, 1980, **19**, 3432 (*In-115 nmr*)

IC-002153

$Br_6Ir^{3\ominus}$
Hexabromoiridate(*III*)(3−), 9CI
[18400-15-2]

$[IrBr_6]^{3\ominus}$ (O_h)

M 671.6 (ion)
Synth. from $Ir^{3\oplus}$(aq.) + excess $Br^{\ominus}$
Tri-K salt: [56604-59-2]. *Potassium hexabromoiridate(III)*
Br_6IrK_3 M 788.9
Spar. sol. H_2O. Obt. as hydrate.

Dwyer, F.P. *et al., J. Proc. R. Soc. N.S.W.*, 1947, **81**, 216 (*synth*)
Botiger, G.L. *et al., Spectrochim. Acta, Part A*, 1972, **28**, 925 (*raman, ir*)
Zipp, S.G. *et al., Inorg. Chim. Acta*, 1975, **14**, 83 (*synth, ir, uv*)

IC-002154

Br_6K_2Tc
Potassium hexabromotechnetate(*IV*) (K_2TcBr_6)
[16903-71-2]

K_2TcBr_6

M 656.5
Synth. by reduction of $TcO_4^{\ominus}$ by HBr/KBr, or by treatment of K_2TcCl_6 with conc. HBr. Dark red cryst. Dec. at 730°. Spar. sol. HBr.

[98478-41-5]

Vinogradov, I.V. *et al., Zh. Neorg. Khim.*, 1978, **23**, 1773; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 975 (*thermal dec*)
Zaitseva, L.L. *et al., Zh. Neorg. Khim.*, 1972, **17**, 2411; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1972, **17**, 1258 (*synth, powder struct*)
Dalziel, J.A.W. *et al., J. Chem. Soc.*, 1958, 4012 (*synth, uv, magnetism, powder struct*)
Schwochau, K. *et al., Z. Naturforsch., A*, 1969, **24**, 403 (*ir*)

$Br_6Mn^{4\ominus}$ IC-002155
Hexabromomanganate(*II*)(4−), 11CI
[34401-68-8]

$[MnBr_6]^{4\ominus}$ (O_h)

M 534.3 (ion)
Tetra-K salt: [38669-04-4]. *Potassium hexabromomanganate(II)* ($K_4(MnBr_6)$)
Br_6K_4Mn M 690.7
Synth. by melting stoichiometric amounts of KBr and $MnBr_2$. Hygroscopic pink cryst.
Tetrakis-Me_2NH_2 salt: [70279-46-8].
Synth. from $[Me_2NH_2]Br$ and $MnBr_2$.

Seifert, H.-J. *et al., Z. Anorg. Allg. Chem.*, 1972, **391**, 302 (*synth, uv, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1978, **C5**, 292 (*rev, bibl*)
Larignon, M. *et al., Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1979, **288**, 119 (*synth, uv-vis*)

$Br_6Mo^{2\ominus}$ IC-002156
Hexabromomolybdate(*IV*)(2−), 9CI
[85192-59-2]

$[MoBr_6]^{2\ominus}$

M 575.3 (ion)
Di-Rb salt: [19639-19-1].
Br_6MoRb_2 M 746.3
Moisture-sensitive olive-green solid.
Di-Cs salt: [19647-78-0].
Br_6Cs_2Mo M 841.1
Prepd. by reaction of $MoBr_4$ or $Mo(CO)_6$ with CsBr in IBr. Moisture-sensitive olive-green solid.
Bis-PPh_3Me salt: [114655-83-3].
Synth. by reaction of $MoBr_4$ with $(PPh_3Me)Br$ in CH_2Br_2. Black-brown cryst. + CH_2Cl_2. Sensitive to hydrolysis.

Edwards, A.J. *et al., J. Chem. Soc.*, 1962, 4643 (*synth*)
Opalovskii, A.A. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 196 (*synth*)
Schmidt, I. *et al., Z. Anorg. Allg. Chem.*, 1988, **556**, 57 (*synth, cryst struct*)

$Br_6Mo_2^{2\ominus}$ IC-002157
Hexabromodimolybdate(2−), 11CI
[108456-70-8]

$[Br_3Mo{\equiv}MoBr_3]^{2\ominus}$

M 671.3 (ion)
Tetrabutylammonium salt: [94554-29-7].
Synth. from $(Bu_4N)Br$ + $Mo(CO)_6$. Brown cryst. (CH_2Cl_2/Et_2O). Diamagnetic.

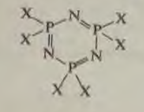
Latorre, J. *et al., Transition Met. Chem.*, 1984, **9**, 447 (*synth*)
Salagre, P.S. *et al., J. Chem. Soc., Dalton Trans.*, 1985, 2263 (*reactions*)

$Br_6Mo_2^{\ominus}$ IC-002158
Hexabromodimolybdate(1−), 11CI
[67954-62-5]

$[Br_3Mo{\equiv}MoBr_3]^{\ominus}$

M 671.3 (ion)
'Ethane-type' struct. proposed with Mo—Mo bond order of 2.5.
Tetrabutylammonium salt: [68024-66-8].
Synth. from $Mo_2(OAc)_4$, Bu_4NBr and HBr. Brown cryst, paramagnetic. Sol. Me_2CO, MeCN, THF. μ_{eff} = 1.5μ_B
Glicksman, H.D. *et al., Inorg. Chem.*, 1978, **17**, 3197 (*synth, uv, ir, esr, pe, deriv*)
Latorre, J. *et al., Transition Met. Chem.*, 1984, **9**, 447.

$Br_6N_3P_3$ IC-002159
2,2,4,4,6,6-Hexabromo-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 9CI, 8CI
Hexabromocyclotriphosphonitrile.
Hexabromocyclotriphosphazene. 2,2,4,4,6,6-Hexabromo-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2,4,4,6,6-Hexabromo-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine
[13701-85-4]



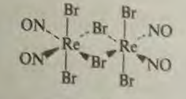
X = Br

M 614.3
Slight chair conformation. Interatomic distances (solid): P—N (mean)157.6, P—Br 216.2 pm; angles: PNP 119.3, 122.4°, NPN 118.5°, BrPBr 102.1°. Synth. from NH_4Br + PBr_3 at 150° in a solvent. Orthorhombic cryst. (C_6H_6 or heptane). Readily sol. C_6H_6, CS_2, $CHCl_3$. Less sol. Et_2O, CCl_4, aliphatic hydrocarbons. Mp 192° (188°). When heated in sealed tube at 220° or subjected to γ irradiation at 80°-150° yields homopolymer.
Homopolymer: Tough, rubbery elastomer between −15° and 270°. Mp ~270°.

[30328-10-0]

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 365 (*rev, bibl*)
Coxon, G.E. *et al., J. Chem. Soc.*, 1967, 1568; 1969, 358 (*ms*)
Manley, T.R. *et al., Spectrochim. Acta, Part A*, 1967, **23**, 149 (*ir, raman*)
Stahlberg, U. *et al., Spectrochim. Acta, Part A*, 1967, **23**, 627 (*ir*)
Lakatos, B. *et al., Acta Chim. (Budapest)*, 1969, **60**, 309 (*uv*)
Zoer, H. *et al., Acta Crystallogr., Sect. B*, 1970, **26**, 1812 (*cryst struct*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 553 (*rev*)
Allcock, H.R., *Phosphorus-Nitrogen Compounds*, Academic Press, London, 1972.
Klosowski, J. *et al., Spectrochim. Acta, Part A*, 1972, **28**, 2189 (*raman*)
Creighton, J.A. *et al., Spectrochim. Acta, Part A*, 1973, **29**, 1077 (*raman*)
Horn, H.G. *et al., Makromol. Chem.*, 1975, **176**, 1359 (*P-31 nmr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 556 (*synth*)
Mason, J. *et al., J. Chem. Soc., Dalton Trans.*, 1977, 2337 (*N-14 nmr*)
Thomas, B. *et al., Z. Chem.*, 1980, **20**, 217 (*N-15 nmr, P-31 nmr*)
Sridharan, K.R. *et al., Polyhedron*, 1983, **2**, 426 (*nqr*)

$Br_6N_4O_4Re_2$ IC-002160
Di-μ-bromotetrabromotetranitrosyldirhenium
Bis(tribromodinitrosylrhenium)
[8415]-11-1]



proposed struct.

M 971.8
Dimeric (from ir evidence) with bromo-bridges and *cis*-NO groups. Synth. from $PPh_4[Re(NO)_2Br_4]$ and $AlBr_3$ in CH_2Br_2. Red-brown powder.

Monomer: Tribromodinitrosylrhenium
$Br_3N_2O_2Re$ M 485.9
Unknown.

Mronga, V.N. *et al., Z. Anorg. Allg. Chem.*, 1982, **491**, 237 (*synth, ir, props*)

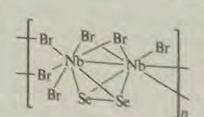
$Br_6Nb^{\ominus}$ IC-002161
Hexabromoniobate(*V*)(1−), 11CI
[32965-80-3]

$[NbBr_6]^{\ominus}$

M 572.3 (ion)
Octahedral. Many salts known.
Cs salt: [21542-23-4]. *Caesium hexabromoniobate(V)*
Br_6CsNb M 705.2
Synth. by heating CsBr + $NbBr_5$ at 110° for 2 weeks.
Me_4N salt: [21999-78-0].
Synth. from $NbBr_5$ and Me_4NBr in hot MeCN. Dark red solid. Forms a mono-CCl_4 solvate.
Ph_4P salt: [79160-81-9].
Synth. from $NbBr_5$ and Ph_4PBr. Dark red cryst.
[22087-55-4]

Brown, D. *et al., J. Chem. Soc. A*, 1967, 247 (*synth, ir, Me_4N salt*)
Horner, S.M. *et al., Inorg. Chem.*, 1968, **7**, 1859 (*synth, ir, uv-vis, Cs salt*)
Mueller, U. *et al., Z. Anorg. Allg. Chem.*, 1981, **473**, 115 (*synth, cryst struct, Ph_4P salt*)

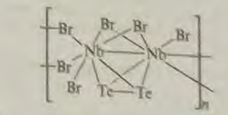
$Br_6Nb_2Se_2$ IC-002162
Niobium(*IV*) bromide selenide ($Nb_2Br_6Se_2$)
Di-μ-bromotetrabromo[μ-(diselenium-Se,Se':Se,Se')]diniobium(IV) *11CI. Hexabromodiselenidodiniobium*(IV)
[86321-92-8]



M 823.1
Synth. by heating the elements to 800° in a sealed ampoule. Air-stable solid with metallic lustre.

Franzen, H.F. *et al., Z. Anorg. Allg. Chem.*, 1983, **497**, 13 (*synth, cryst struct*)

$Br_6Nb_2Te_2$ IC-002163
Niobium(*IV*) bromide telluride ($Nb_2Br_6Te_2$)
Di-μ-bromotetrabromo[μ-(ditellurium-Te,Te':Te,Te')]diniobium(IV), *11CI. Hexabromoditelluridodiniobium*(IV)
[86437-64-1]



M 920.4
Synth. by heating the elements in a sealed ampoule at 800°. Solid with metallic lustre, stable to H_2O and O_2.

Franzen, H.F. *et al., Z. Anorg. Allg. Chem.*, 1983, **497**, 13 (*synth, cryst struct*)

IC-002164

$Br_6Np^{2\ominus}$

Hexabromoneptunate(*IV*)(2−)

[91630-85-2]

$[NpBr_6]^{2\ominus}$ (O_h)

M 716.4 (ion)

Di-Cs salt: [65464-94-0].
Br_6Cs_2Np M 982.2
Yellow-brown microcryst. K_2PtCl_6 struct.

Bis-Et_4N salt: Bright yellow solid.

Ryan, J.L. *et al, Mol. Phys.*, 1963, **7**, 17 (*synth, uv-vis*)
Magerlin, M. *et al, Inorg. Nucl. Chem. Lett.*, 1977, **13**, 529 (*synth, cryst struct*)
Fuger, J., *J. Phys. Colloq.*, 1979, 307 (*rev*)

IC-002165

Br_6OSi_2

Hexabromodisiloxane, 9Cl

$Br_3SiOSiBr_3$

M 551.5
Synth. by oxidation of $SiBr_4$ or by the reaction of O_2 and Br_2 with Si. Colourless liq. or tabular cryst. Mp 27.9°. Bp_{13} 118°.

Schumb, W.C. *et al, J. Am. Chem. Soc.*, 1937, **59**, 261 (*synth*)
Buerger, H. *et al, Z. Chem.*, 1968, **8**, 256 (*ir, raman*)

IC-002166

$Br_6Os^{3\ominus}$

Hexabromoosmate(*III*)(3−)

[44442-35-5]

$[OsBr_6]^{3\ominus}$

M 669.6 (ion)
Synth. by electrolytic reduction of solns. of $[OsBr_6]^{2\ominus}$.

Tris(ethylenediamine)cobalt(III) salt: [99326-42-8].
Synth. from $Na_2[OsBr_6]$ in dil. HBr with Ag followed by addition of $Co(en)_3Br_3$. μ_{eff} = 1.67μ_B at 298K.

Crowell, W.R. *et al, J. Am. Chem. Soc.*, 1938, **60**, 1105 (*synth, uv, electrochem*)
Meir, H. *et al, Mikrochim. Acta*, 1976, **I**, 183 (*electrochem*)
Campbell, N.J. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1673 (*synth, ir, raman*)

IC-002167

$Br_6Os^{2\ominus}$

Hexabromoosmate(*IV*)(2−)

[16920-04-0]

$[OsBr_6]^{2\ominus}$ (O_h)

M 669.6 (ion)
Many salts known, made by reaction of OsO_4 and HBr in the presence of the appropriate cation. Grp. I salts have cubic K_2PtCl_6 struct. Used as a starting material for many other osmium compounds. Ir ν 227, 122 cm^{-1}. Raman 210.6, 169.2, 100 cm^{-1}.

Di-Na salt: Shining brown-black, metallic prisms (deep purple in soln.).
Di-K salt: [16903-69-8].
Brown-black, coppery coloured powder.
Di-H compd.: [48016-85-9].
Synth. from OsO_4 and HBr.
Di-NH_4 salt: [24598-62-7].
Synth. by refluxing OsO_4 and HBr for 2 hr., followed by addition of NH_4Br and EtOH. Minute black cubes. Sol. warm glycerol, ethylene glycol; spar. sol. cold H_2O to give red solns., dec. in hot H_2O; insol. EtOH, MeOH.

Inorg. Synth., 1957, **5**, 204

Jörgensen, C.K., *Mol. Phys.*, 1959, **2**, 309 (*uv*)
Jörgensen, C.K., *Prog. Inorg. Chem.*, 1970, **12**, 101 (*rev, uv*)
Bottger, G.L. *et al, Spectrochim. Acta*, 1972, **28**, 925 (*ir*)
Fergusson, J.E. *et al, Aust. J. Chem.*, 1974, **27**, 661
Bosworth, Y.M. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1749 (*ir, uv*)
Ikeda, K.I. *et al, Inorg. Chem.*, 1978, **17**, 2698 (*uv*)
Homborg, H. *et al, Z. Anorg. Allg. Chem.*, 1980, **460**, 17 (*raman*)
Linko, I.V. *et al, Zh. Neorg. Khim.*, 1983, **28**, 1520; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 857 (*pe*)

IC-002168

$Br_6Os^{\ominus}$

Hexabromoosmate(*V*)(1−)

[86365-51-7]

$[OsBr_6]^{\ominus}$

M 669.6 (ion)
Dec. has so far precluded isolation of a salt of this ion. Synth. from $[Et_4N]_2[OsBr_6]$ and PbO_2 in MeCN. λ_{max} 626, 550, 489 nm.

Magnuson, R.H., *Inorg. Chem.*, 1984, **23**, 387 (*synth, electrochem, uv*)

IC-002169

$Br_6Pb^{4\ominus}$

Hexabromoplumbate(*II*)(4−)

$[PbBr_6]^{4\ominus}$

M 686.6 (ion)
Tetra-Cs salt: [15655-27-3]. *Caesium lead bromide* (Cs_4PbBr_6)
Br_6Cs_4Pb M 1218.2
From $PbBr_2$ + CsBr. White rhombohedral cryst.

Wells, H.L., *Z. Anorg. Allg. Chem.*, 1893, **3**, 195 (*synth*)
Il'yasov., *et al, Zh. Neorg. Khim.*, 1966, **11**, 1986; *CA*, 1964, **65**, 14513d (*phase diagram*)
Cygler, M. *et al, Acta Univ. Lodz., Ser. 2*, 1976, **13**, 75; *CA*, 1977, **87**, 109837a (*cryst struct*)

IC-002170

$Br_6Pd^{2\ominus}$

Hexabromopalladate(*IV*)(2−)

[32627-95-5]

$[PdBr_6]^{2\ominus}$ (O_h)

M 585.8 (ion)
Possible anti-tumour props. investigated. Ir ν_{Pd-Br} ~ 250 cm^{-1}.

Di-K salt: [16919-74-7]. *Potassium hexabromopalladate*(IV) (K_2PdBr_6)
Br_6K_2Pd M 664.0
Black cryst. K_2PtCl_6 struct. Dec. to K_2PdBr_4 >250°.

Di-Rb salt: [19121-82-5].
Br_6PdRb_2 M 756.7
Brown to black solid. K_2PtCl_6 struct. Dec. to Rb_2PdBr_4 >260°.

Di-Cs salt: [19121-77-8].
Br_6Cs_2Pd M 851.6
Brown to black solid. K_2PtCl_6 struct. Dec. to Cs_2PdBr_4 >240°.

Di-NH_4 salt: [61104-71-0].
Black-red brown cryst. K_2PtCl_6 struct.

Bis-$MeNH_3$ salt: [70366-03-9].
Brown solid. Similar compds. obt. for other primary amines.

Bis[ethylenediammonium(1+)] salt: [64593-52-8].
Brown solid. Similar salts prepd. for other amines.

Guthner, A. *et al, Chem. Ber.*, 1905, **38**, 2385 (*synth*)

Ketelaar, J.A.A. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1938, **57**, 964 (*struct, synth*)
Sharpe, A.G., *J. Chem. Soc.*, 1953, 4177 (*synth, cryst struct*)
Brown, D.H. *et al, J. Chem. Soc. A*, 1967, 100 (*ir*)
Hendra, P.J. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 1635 (*raman*)
Shuhochkin, L.K. *et al, Zh. Neorg. Khim.*, 1976, **21**, 2567; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1413 (*thermal dec*)
Perison, J.B. *et al, Spectrochim. Acta, Part A*, 1977, **33**, 487 (*ir, raman*)
Kume, Y. *et al, J. Magn. Reson.*, 1979, **33**, 331 (*nqr*)
Knop, O. *et al, J. Chem. Soc., Faraday Trans. 2*, 1981, **77**, 811 (*ir, struct*)
Mohan, S. *et al, Indian J. Phys., B*, 1982, **56**, 91 (*ir*)

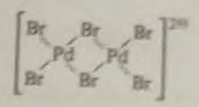
IC-002171

$Br_6Pd_2^{2\ominus}$

Di-μ-bromotetrabromodipalladate(*II*)(2−), 8Cl

Hexabromodipalladate(II)(2−)

[33887-55-7]



M 692.2 (ion)
Probable struct. shown. Synth. from Tetrabromopalladate(*II*)(2−), IC-002064 + $R_4N^{\oplus}Br^{\ominus}$ (R = Et, Bu etc.).

Bis-Et_4N salt: [18535-42-7].
Brown plates. Sol. CH_2Cl_2, Me_2CO, $PhNO_2$.

Bis-tetrabutylammonium salt: [21620-72-4].
Sol. CH_2Cl_2.

Harris, C.M. *et al, J. Chem. Soc.*, 1958, 3697 (*synth, elec cond*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1483 (*synth, ir, raman*)
Lobanova, O.A. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 1577 (*uv*)

IC-002172

$Br_6Pr^{3\ominus}$

Hexabromopraseodymate(*III*)(3−)

[29753-85-3]

$[PrBr_6]^{3\ominus}$ (O_h)

M 620.3 (ion)

Tri-Na salt: [36423-39-9]. *Sodium hexabromopraseodymate*(III)
Br_6Na_3Pr M 689.3
Green cryst. Mp 375°

Di-Cs, Li salt: [69208-02-2].
Br_6Cs_2LiPr M 893.0
Green cryst. Possesses elpasolite struct.

Di-Cs, Na salt
Br_6Cs_2NaPr M 909.1
Green cryst. Possesses elpasolite struct. at > −17°

Tri-Cs salt: [36423-44-6]. *Caesium hexabromopraseodymate*(III)
Br_6Cs_3Pr M 1019.0
Green cryst. Mp 749°

Tris-Ph_3PH salt: Deliquescent green cryst. + $1Ph_3PHBr$.

Ryan, J.L. *et al, J. Phys. Chem.*, 1966, **70**, 2845 (*synth, uv-vis*)
Ryan, J.L., *Inorg. Chem.*, 1969, **8**, 2053 (*synth, uv-vis*)
Vogel, G., *Z. Anorg. Allg. Chem.*, 1972, **388**, 43 (*synth*)
Meyer, G. *et al, Z. Naturforsch., B*, 1978, **33**, 1476 (*synth*)
Inorg. Synth., 1983, **22**, 11 (*synth*)

IC-002173

$Br_6Pt^{2\ominus}$

Hexabromoplatinate(*IV*)(2−), 8Cl

[16871-55-9]

$[PtBr_6]^{2\ominus}$ (O_h)

M 674.5 (ion)
Many salts with organic or complex cations known. Many studies of reaction mechanisms. Synth. from Pt + Br_2 + HBr, followed by salt of required cation.

Di-Na salt: [39277-13-9]. *Sodium hexabromoplatinate*(IV) (Na_2PtBr_6)
Red solid. Sol. H_2O.

Di-K salt: [16920-95-7]. *Potassium hexabromoplatinate*(IV) (K_2PtBr_6)
Commercially available. Orange-red solid. Sol. H_2O.
▷ TP1389000

Delmas, M. *et al, Comptes Rend. Hebd. Seances Acad. Sci. Sect. B*, 1967, **264**, 1724 (*ir, raman*)
Grundy, H.D. *et al, Can. J. Chem.*, 1970, **48**, 1103 (*struct*)
Fleming, G.N. *et al, J. Am. Chem. Soc.*, 1970, **92**, 3177 (*pe, xsd*)
Bosworth, Y.M. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1749 (*raman*)
Inorg. Synth., 1979, **19**, 2 (*synth*)
Kemmitt, S.J.S. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 2503 (*Pt-195 nmr*)

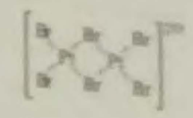
IC-002174

$Br_6Pt_2^{2\ominus}$

Di-μ-bromotetrabromodiplatinate(*II*)(2−), 8Cl

Hexabromodiplatinate(II)(2−)

[31826-84-3]



M 869.5 (ion)
Square planar $PtBr_4$ units. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + $Br^{\ominus}$ + R_4NBr, or from $PtBr_2$ + R_4NBr in DMF.

Bis-Et_4N salt: [18475-81-5].
Yellow-brown plates. Sol. Me_2CO, $PhNO_2$.

Bis-tetrabutylammonium salt: [51514-30-0].
Dark green solid. Sol. Me_2CO, CH_2Cl_2. Mp 138–139°.

Harris, C.M. *et al, J. Chem. Soc.*, 1958, 3697 (*synth, struct*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1298, 1476, 1483 (*synth, ir, raman*)
Russell, D.R. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2550 (*struct*)
Martin, D.S. *et al, Inorg. Chem.*, 1976, **15**, 669 (*uv*)

IC-002175

$Br_6Pu^{3\ominus}$

Hexabromoplutonate(*III*)(3−)

$[PuBr_6]^{3\ominus}$

M 718.4 (ion)

Tris-Ph_4P salt: [18372-73-1].
Air-sensitive solid.

Ryan, J.L., *Adv. Chem. Ser.*, 1967, **71**, 133

IC-002176

$Br_6Pu^{2\ominus}$

Hexabromoplutonate(*IV*)(2−)

$[PuBr_6]^{2\ominus}$

M 718.4 (ion)

Di-Cs salt: [7034]-24-1]. *Caesium hexabromoplutonate*(IV)

Br_6Cs_2Pt M 984.2
Red solid.
Bis-Et₄N salt: Dark red cryst. Sol. org. solvs.
Ryan, J.L. *et al, Mol. Phys.*, 1965, **7**, 17.
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, **C**, 151 (*rev*)
Fuger, J., *J. Phys. Colloq.*, 1979, 207.
Fuger, J., *ACS Symp. Ser.*, 1983, **216**, 75 (*rev*)

IC-002177

$Br_6Re^{2\ominus}$

Hexabromorhenate(*IV*)(2−), 9Cl

[16871-51-5]

$[ReBr_6]^{2\ominus}$

M 665.6 (ion)
Octahedral anion; Re—Br 248 pm (K salt). Synth. from $ReO_4^{\ominus}$, HBr aq. and H_3PO_2 in presence of suitable cation. Also formed by prolonged treatment of $ReCl_6^{2\ominus}$ with conc. HBr. Red-brown solns: stable in HBr aq. Readily hydrol.
Di-K salt: [16903-70-1]. *Potassium hexabromorhenate*(IV) (K_2ReBr_6)
Br_6K_2Re M 743.8
Dark red cryst. (HBr aq.). K_2PtCl_6 type structure.
Di-Cs salt: [17475-93-3].
Br_6Cs_2Re M 931.4
Reddish-brown powder; colour depends on state of division. K_2PtCl_6 type structure.
Di-Ag(I) salt: [27865-77-6].
Ag_2Br_6Re M 881.3
Synth. by precipitation from HNO_3 soln. of K_2ReBr_6. Solid. Dec. on heating to $ReBr_3$.
Di-NH_4 salt: [21135-41-1].
Dark red cryst. (HBr aq.). K_2PtCl_6 type structure.

Inorg. Synth., 1963, **7**, 189 (*synth, props*)
Grundy, H.D. *et al, Can. J. Chem.*, 1970, **48**, 151 (*cryst struct*)
Rouschias, G., *Chem. Rev.*, 1974, **74**, 552 (*synth, props, rev, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1626 (*synth*)
Hauck, J. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2124 (*cryst struct, ir, props*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, 172 (*rev, bibl*)

IC-002178

$Br_6Rh^{3\ominus}$

Hexabromorhodate(*III*)(3−), 9Cl

$[RhBr_6]^{3\ominus}$

M 582.3 (ion)
2,2',2"-Triammoniotriethylamine salt trihydrate: [56604-58-1].
Red-brown solid. Stable beyond 300°.

Zipp, S.G. *et al, Inorg. Chim. Acta*, 1975, **14**, 83 (*synth, ir, uv*)

IC-002179

$Br_6Ru^{3\ominus}$

Hexabromoruthenate(*III*)(3−), 9Cl

[21159-26-2]

$[RuBr_6]^{3\ominus}$ (O_h)

M 580.4 (ion)
Only isolated in the solid state as two very unusual salts. Easily oxidized in soln. to $[RuBr_6]^{2\ominus}$. V. sol. aq. HBr. The uv spectra reported in the literature strongly resemble those of the oxidized product $[RuBr_6]^{2\ominus}$ and must be treated with suspicion.
Anilinium salt; double salt with anilinium bromide (1:3): [31304-66-2].
Brown monoclinic cryst. Formulated as $[PhNH_3]_3[RuBr_6]Br_3$. Ru—Br 251.4 pm. μ_{eff} = 2.09μ_B. Ir ν_{RuBr} 240, 232 cm^{-1}.
Tris(2-aminoethylammonium(3+) salt: hydrogen bromide complex: [38782-87-5].
Formulated as $[N(CH_2CH_2NH_3)_3][RuBr_6]$·HBr. Ir ν_{RuBr} 240 cm^{-1}; μ_{eff} = 2.01μ_B.

Joergensen, C.K., *Acta Chem. Scand.*, 1956, **10**, 518 (*uv*)
Joergensen, C.K., *Mol. Phys.*, 1959, **2**, 309 (*uv*)
Drew, M.G.B. *et al, Inorg. Nucl. Chem. Lett.*, 1971, **7**, 59 (*synth, uv, cryst struct, μ_{eff}*)
Gaylor, J.R. *et al, Inorg. Chem.*, 1972, **11**, 2551 (*synth, uv, ir, μ_{eff}*)
Corrigan, D.A. *et al, J. Chem. Phys.*, 1979, **70**, 5676 (*esr*)
Campbell, N.J. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1673 (*ir, raman*)

IC-002180

$Br_6Ru^{2\ominus}$

Hexabromoruthenate(*IV*)(2−)

[57448-76-7]

$[RuBr_6]^{2\ominus}$ (O_h)

M 580.4 (ion)
Prepd. by oxidation of $RuBr_3$ complexes in aq. HBr by Br_2. Sol. aq. HBr.
Di-K salt: [52637-67-9].
Br_6K_2Ru M 658.6
Purple-black cubic cryst. μ_{eff} 2.84μ_B; Ir ν_{RuBr} 248 cm^{-1}.
Di-Rb salt: [52637-69-1].
Br_6Rb_2Ru M 751.4
Purple-black cubic cryst. μ_{eff} 2.81μ_B; Ir ν_{RuBr} 246 cm^{-1}.
Di-Cs salt: [52637-70-4].
Br_6Cs_2Ru M 846.3
Purple-black cubic cryst. Ir ν_{RuBr} 243 cm^{-1}.
Di-NH_4 salt: [52637-68-0].
$Br_6H_8N_2Ru$ M 616.5
Purple-black cubic cryst. Ir ν_{RuBr} 248 cm^{-1}.
Bis-tetrabutylammonium salt: Purple-black cryst.

Howe, J.L., *J. Am. Chem. Soc.*, 1904, **26**, 942 (*synth*)
Earnshaw, A. *et al, J. Chem. Soc.*, 1961, 3132 (*magnetism*)
Johanneson, R.B. *et al, Inorg. Chem.*, 1963, **2**, 67 (*magnetism*)
Pantani, F. *et al, Ric. Sci. Rend. Sez. A*, 1964, **4**, 535 (*uv*)
Fergusson, J.E. *et al, Aust. J. Chem.*, 1974, **27**, 661 (*struct, ir*)
Collingwood, J.C. *et al, Mol. Phys.*, 1975, **30**, 469 (*uv*)
Fergusson, J.E. *et al, Aust. J. Chem.*, 1978, **31**, 497 (*synth*)
Clark, R.J.H. *et al, Mol. Phys.*, 1984, **52**, 859 (*uv, raman*)
Campbell, N.J. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1673 (*ir, raman*)
Appleby, D. *et al, Nature (London)*, 1986, **323**, 614 (*uv*)

IC-002181

$Br_6Sb^{\ominus}$

Hexabromoantimonate(*V*)(1−), 8CI

[22994-42-9]

$[SbBr_6]^{\ominus}$

M 601.1 (ion)
Me_4N salt: [30454-59-2].
$C_4H_{12}Br_6NSb$ M 675.3
Carmine-red cryst.
Et_4N salt: [30454-67-2].
Synth. from $Et_4N[SbBr_4]$ + Br_2/HBr aq. V. dark red-brown cryst. Tetragonal system with Sb in distorted $SbBr_6$ anions.
Tetrabutylammonium salt: [63750-31-2].
Deep red-brown solid. Stable to air and resistant to hydrol.
H compd.: see *Hydrogen hexabromoantimonate*(V)(1−), *IC-002141*

Gmelin Handbook Inorg. Chem., Syst. No. 18, 1949, 484 (*rev, bibl*)

Hackert, M.L. *et al, Inorg. Chem.*, 1971, **10**, 1075 (*cryst struct*)
Adams, C.J. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 1829 (*synth, ir, raman*)
Kidd, R.G. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 861 (*nmr*)
Clark, R.J.H. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 790 (*props, raman*)
Goetz-Grandmont, G.J. *et al, Z. Anorg. Allg. Chem.*, 1983, **496**, 40 (*synth*)

Br_6Si_2

Hexabromodisilane, 9CI IC-002182

Silicon bromide (Si_2Br_6), 8CI

[13517-13-0]

$Br_3SiSiBr_3$

M 535.5
Synth. by the action of Br_2 on a Ca—Si alloy at 180-200°. Plates or prisms. Sol. CCl_4, $CHCl_3$, CS_2, C_6H_6, $SiCl_4$, $SiBr_4$. Mp 95°. Bp 265°.

Inorg. Synth., 1946, **2**, 98 (*synth*)
Hoefler, F. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 819 (*ir, raman*)

$Br_6Sn^{4\ominus}$

Hexabromostannate(*II*)(4−) IC-002183

$[SnBr_6]^{4\ominus}$

M 598.1 (ion)
Tetra-Cs salt: [57373-75-8]. *Caesium tin bromide (Cs_4SnBr_6)*
Br_6Cs_4Sn M 1129.7
From the molten CsBr/$SnBr_2$ system. Freshly prepd. samples are black but turn yellow, then white in moist air. Contains discrete $[SnBr_6]^{4\ominus}$ anions.

Donaldson, J.D. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1500 (*synth, mössbauer, cryst struct*)
Andrews, R.H. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 767 (*synth, cryst struct, mössbauer*)

$Br_6Sn^{2\ominus}$

Hexabromostannate(*IV*)(2−), 9CI IC-002184

Bromostannate(IV)

[16871-49-1]

$[SnBr_6]^{2\ominus}$ (O_h)

M 598.1 (ion)
General synth. from $SnBr_4$ + MBr in conc. HBr. Many salts are known with alkali metal and alkylammonium cations.
Di-K salt: [17362-95-7].
Br_6K_2Sn M 676.3
Cryst. K_2PtCl_6 struct.
Di-Rb salt: [17362-96-8].
Br_6Rb_2Sn M 769.0
Cryst. K_2PtCl_6 struct.
Di-Cs salt: [17362-97-9].
From CsBr + $SnBr_4$. Cryst. K_2PtCl_6 struct.
Di-NH_4 salt: [16925-34-1].
Cryst.
Bis-tetrabutylammonium salt: Yellow needles.

Raymann, B. *et al, Justus Liebigs Ann. Chem.*, 1884, **223**, 323 (*synth*)
Costeanu, C.I., *Ber., B*, 1927, **60**, 1312 (*synth*)
Ketelaar, J.A.A. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1937, **56**, 907 (*cryst struct, NH_4, H, Rb, Cs salts*)
Debeau, M. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1967, **264**, 1724 (*ir*)
Fergusson, J.E. *et al, Aust. J. Chem.*, 1974, **27**, 661 (*cryst struct*)
Bosworth, Y.M. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1749 (*raman*)
Donaldson, J.D. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1980 (*ir, raman*)
Higashi, T. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 144 (*cryst struct, K salt*)
Dillon, K.B. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1245 (*synth, Sn-119 nmr*)

$Br_6Ta^{2\ominus}$

Hexabromotantalate(*IV*)(2−), 11CI IC-002185

[65452-27-9]

$[TaBr_6]^{2\ominus}$ (O_h)

M 660.3 (ion)
Di-Rb salt: [97882-06-9].
Br_6Rb_2Ta M 831.3
Synth. by melting RbBr + $TaBr_4$ in a sealed tube. ΔH_f° −1330 kJ mol^{-1}.
Di-Cs salt: [21542-19-8].
Br_6Cs_2Ta M 926.1
Synth. by heating solid CsI and $CsTaBr_6$ in a sealed tube at 310°. Dark blue-green solid. Weakly paramagnetic. Ir ν_3 217, ν_4 109 cm^{-1}.
Horner, S.M. *et al, Inorg. Chem.*, 1968, **7**, 1859 (*synth, uv-vis, ir, magnetism*)
Westland, A.D., *Thermochim. Acta*, 1985, **87**, 29 (*synth, thermochem*)

$Br_6Ta^{\ominus}$

Hexabromotantalate(*V*)(1−), 11CI IC-002186

[32965-79-0]

$[TaBr_6]^{\ominus}$ (O_h)

M 660.3 (ion)
Cs salt: [21542-20-1].
Br_6CsTa M 793.2
Synth. by heating a mixture of $TaBr_5$ and CsBr to 110°. Yellow solid. Other alkali metal salts may be made in the same way.
Me_4N salt: [22087-56-5].
Synth. by reaction of $TaBr_5$ and $[Me_4N]Br$ in MeCN. Forms a CCl_4 (1:1) adduct.
Ph_4P salt: [79169-58-7].
Synth. from $TaBr_5$ and $[Ph_4P]Br$.

Brown, D. *et al, J. Chem. Soc. A*, 1967, 247 (*synth, uv-vis, ir*)
Horner, S.M. *et al, Inorg. Chem.*, 1968, **7**, 1859 (*synth, uv-vis, ir*)
Mueller, U. *et al, Z. Anorg. Allg. Chem.*, 1981, **473**, 115 (*synth, cryst struct, reactions*)

$Br_6Tc^{2\ominus}$

Hexabromotechnetate(*IV*)(2−) IC-002187

[19443-24-4]

$[TcBr_6]^{2\ominus}$ (O_h)

M 578.3 (ion)
Obt. by reduction of $TcO_4^{\ominus}$ by cold conc. HBr. Useful starting material for prep. of Tc^{IV} complexes. Readily hydrol. μ_{eff} = 3.94μ_B.
Di-K salt: see *Potassium hexabromotechnetate*(IV) (K_2TcBr_6), *IC-002154*
Mg salt: [110873-73-9].
Br_6MgTc M 602.6
Reddish-brown cryst., dec. at *ca.* 450°. Sol. warm HBr; insol. $CHCl_3$, CCl_4, C_6H_6.
Ca salt: [88608-68-8].

Br_6CaTc M 618.4
Red cryst., dec. above 380°. Sol. HBr; spar. sol. Me_2CO; insol. CCl_4, $CHCl_3$.
Sr salt: [110873-74-0].
Br_6SrTc M 665.9
Reddish-brown cryst., dec. at *ca.* 350°. Sol. warm HBr; insol. $CHCl_3$, CCl_4, C_6H_6.
Ba salt: see *Barium hexabromotechnetate*(IV), *IC-001296*
Pb salt: [105204-91-9].
Br_6PbTc M 785.5
Synth. from $Pb(TcO_4)_2$ (from $PbCO_3$ + $HTcO_4$) and $PbBr_2$ and HBr. Red-brown cryst., isostructural with $BaTcBr_6$, hydrol. by H_2O. Insol. EtOH, CCl_4.
Bis-NH_4 salt: see *Diammonium hexabromotechnetate*(IV) ($(NH_4)_2TcBr_6$), *IC-002147*
Bis-tetrabutylammonium salt: [112816-20-3].
Synth. by metathesis from K_2TcBr_6. Red-brown cryst. (Me_2CO/hexane).

[55266-21-2, 71128-59-1]

Dalziel, J.A.W. *et al*, *J. Chem. Soc.*, 1958, 4012 (*synth, magnetism*)
Joergenson, C.K. *et al*, *Z. Naturforsch., A*, 1965, **20**, 1276 (*uv*)
Schwochau, K., *Z. Naturforsch., A*, 1965, **20**, 1286 (*stability, ligand exchange kinetics*)
Ossicini, L., *Ric. Sci.*, 1967, **37**, 655 (*hydrol*)
Zaitseva, L.L. *et al*, *Zh. Neorg. Khim.*, 1973, **18**, 2410; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **18**, 1276 (*synth, powder struct*)
Verdonck, E. *et al*, *Inorg. Chim. Acta*, 1977, **23**, 67 (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, *Suppl. vol.* 2, 1983, 115, 193.
Zaitseva, L.L. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 3050; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1729 (*Ca salt, synth, dta, tga, powder struct*)
Thomas, R.W. *et al*, *Inorg. Chem.*, 1985, **24**, 1472 (*exafs*)
Zaitseva, L.L. *et al*, *Zh. Neorg. Khim.*, 1986, **31**, 2184; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1986, **31**, 1260 (*Pb salt, synth, ir, dta, tga, powder struct*)
Huber, E.W. *et al*, *Inorg. Chem.*, 1987, **26**, 3718 (*electrochem*)
Zaitseva, L.L. *et al*, *Zh. Neorg. Khim.*, 1987, **32**, 1606; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1987, **32**, 959 ($M^{2\oplus}$ *salts*)
Colin, M. *et al*, *J. Radioanal. Nucl. Chem.*, 1988, **120**, 175 (*aquation, photol, uv*)
Makarov, L.L. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1989, **307**, 644 (*xrf*)
March, J.G. *et al*, *J. Radioanal. Nucl. Chem.*, 1989, **132**, 293 (*ligand exchange in non-aq soln*)

$Br_6Th^{2\ominus}$

Hexabromothorate(*IV*)(2−) IC-002188
[44490-06-4]

$ThBr_6^{2\ominus}(O_h)$

M 711.4 (ion)
Di-K salt: [59570-90-0]. *Potassium hexabromothorate*(IV). *Dipotassium hexabromothorate*(2−)
Br_6K_2Th M 789.6
White cryst. Raman ν_{Th-Br} 175 cm^{-1}.
Di-Rb salt: [59570-91-1]. *Rubidium hexabromothorate*(IV). *Dirubidium hexabromothorate*(2−)
Br_6Rb_2Th M 882.3
White cryst.
Di-Cs salt: [59570-92-2]. *Caesium hexabromothorate*(IV). *Dicaesium hexabromothorate*(2−)
Br_6Cs_2Th M 977.2
White cryst. Raman ν_{Th-Br} 198 cm^{-1}.
Bis-Me_4N salt: [12074-06-5].
White cryst. Sol. MeCN. Ir ν_{Th-Br} 179 cm^{-1}. Has fcc struct.
Bis-Et_4N salt: [22003-86-7].
White cryst. Sol. MeCN. Ir ν_{Th-Br} 177 cm^{-1}.

Brown, D., *J. Chem. Soc. A*, 1966, 766 (*synth, ir, struct*)
Inorg. Synth., 1970, **12**, 229 (*synth*)
Ribas Bernat, J.G. *et al*, *Ion* (*Madrid*), 1976, **36**, 11 (*synth*)
Mehta, M.L., *Monatsh. Chem.*, 1979, **110**, 857 (*ir, raman*)
Gershanovich, A.Yu. *et al*, *Radiokhimiya*, 1981, **23**, 211; *CA*, **95**, 53972 (*synth*)
Tuck, D.G. *et al*, *Can. J. Chem.*, 1982, **60**, 2579 (*synth*)
Westland, A.D. *et al*, *Can. J. Chem.*, 1983, **61**, 1573 (*synth, raman, bond energies*)

$Br_6Ti^{2\ominus}$

Hexabromotitanate(*IV*)(2−), 11Cl IC-002189
[27709-79-1]

$[TiBr_6]^{2\ominus}$

M 527.3 (ion)
Bis-Et_4N salt: [21336-51-6].
Synth. by mixing CH_2Cl_2 solns. of Et_4NBr and $TiBr_4$ or by electrochemical oxidation of Ti in the presence of bromine. Red solid (CH_2Cl_2).
Bis(thiotrithiazyl) salt: [64094-16-2].
Synth. from $TiBr_4$ and S_4N_3Br in CH_2Cl_2. Orange solid.

Clark, R.J.H. *et al*, *Inorg. Chem.*, 1968, **7**, 1603 (*synth, ir, raman, Et_4N salt*)
Paul, R.C. *et al*, *J. Indian Chem. Soc.*, 1976, **53**, 1228 (*synth, S_4N_3 salt*)
Habeeb, J.J. *et al*, *Can. J. Chem.*, 1977, **55**, 3882 (*electrochem synth, Et_4N salt*)
Hao, N. *et al*, *J. Magn. Reson.*, 1982, **50**, 50 (*Ti-47 nmr, Ti-49 nmr*)
Mohan, S. *et al*, *Indian J. Phys., B*, 1983, **57**, 420 (*theory, ir*)

$Br_6Tl^{3\ominus}$

Hexabromothallate(*III*)(3−) IC-002190
[44490-91-7]

$[TlBr_6]^{3\ominus}$ (O_h)

M 683.8 (ion)
Synth. from aq. sol. of $TlBr_3$ and required bromide salts. Yellow salts.
▷ Toxic.
Cs, Di-H salt: [67928-10-3].
Br_6CsH_2Tl M 818.7
Obt. in nitrobenzene soln.
Tri-Rb salt: [15168-67-9].
Br_6Rb_3Tl M 940.2
Solid + $\frac{8}{7}$ H_2O.

Spiro, T.G., *Inorg. Chem.*, 1967, **6**, 569 (*ir, raman*)
Studnicova, M., *Collect. Czech. Chem. Commun.*, 1978, **43**, 719 (*synth*)
Glaser, J. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 6642 (*Tl-205 nmr*)
Geldard, J.F. *et al*, *Spectrochim. Acta, Part A*, 1987, **43**, 439 (*ir*)

Br_6Tl_4

Thallium(*I*) hexabromothallate(*III*) IC-002191
Thallium bromide (Tl_4Br_6)

$Tl_3[TlBr_6]$

M 1296.9
Intermed. in oxid. of TlBr by conc. HNO_3. Synth. from TlBr + Br_2.
▷ Highly toxic.

Batsanov, S.S. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1964, 91.

$Br_6U^{3\ominus}$

Hexabromouranate(*III*)(3−) IC-002192
[87652-39-9]

$UBr_6^{3\ominus}$

M 717.4 (ion)
Na, Di-K salt: [86730-42-9].
Br_6K_2NaU M 818.6
Violet cryst. 6-Coord. with the Elpasolite struct.
Tri-K salt: [53513-85-2].
Br_6K_3U M 834.7
Violet cryst. Mp 587°. Cubic struct.
Na, Di-Rb salt:
Br_6NaRb_2U M 911.3
Violet cryst. 6-Coord. Elpasolite struct.
Tri-Rb salt: [53513-87-4].
Br_6Rb_3U M 973.8
Dark violet cryst. Mp 695°. Cubic struct.
Na, di-Cs salt: [86730-43-0].
Br_6Cs_2NaU M 1006.2
Violet cryst. 6-Coord. Elpasolite struct.
Tri-Cs salt: [53513-89-6].
Br_6Cs_3U M 1116.1
Dark violet cryst. Mp 758°. Cubic struct.

Vdovenko, V.M. *et al*, *Radiokhimiya*, 1974, **16**, 369 (*synth, struct*)
Suglobova, I.G. *et al*, *Radiokhimiya*, 1978, **20**, 352; *Sov. Radiochem.* (*Engl. Transl.*), 1978, **20**, 1302 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 55 *Suppl. Vol.*, 1981, **C9**, 132 (*bibl, rev*)
Aurov, N.A. *et al*, *Radiokhimiya*, 1983, **25**, 366; *Sov. Radiochem.* (*Engl. Transl.*), 1983, **25**, 348 (*synth, struct*)

$Br_6U^{2\ominus}$

Hexabromouranate(*IV*)(2−) IC-002193
[40530-91-4]

$UBr_6^{2\ominus}$ (O_h)

M 717.4 (ion)
Di-Cs salt: [21082-89-3]. *Caesium hexabromouranate*(IV). *Dicaesium hexabromouranate*(2−)
Br_6Cs_2U M 983.2
Green cryst.
Bis-Me_4N salt: Green solid. Sol. MeCN. Ir ν_{UBr} 181 cm^{-1}.
Bis-Et_4N salt: [12080-72-7].
Green cryst. Sol. MeCN. Ir ν_{UBr} 178 cm^{-1}.
Bis-ethyltriphenylphosphonium salt: [66683-81-6].
Green(?) cryst. Sol. MeCN.
Bis-butyltriphenylphosphonium salt: Green cryst. Sol. MeCN. Mp 256-258°.
Bis-Ph_4P salt: Cryst. + 4MeCN.
Bis(2,5-dimethyl-3,3a,4-trithia-1-azapentalenium) salt: Red-brown cryst. Ir ν_{UBr} 229 cm^{-1}.

Ryan, J.L. *et al*, *Mol. Phys.*, 1963, **7**, 17 (*synth, uv-vis*)
Day, J.P. *et al*, *J. Chem. Soc. A*, 1966, 197 (*synth, magnetism, uv-vis*)
Brown, D. *et al*, *J. Chem. Soc. A*, 1966, 766 (*synth, ir*)
Inorg. Synth., 1974, **15**, 236 (*synth*)
Caira, M.R. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 1116 (*synth, cryst struct*)
Kepert, D.L. *et al*, *Aust. J. Chem.*, 1983, **36**, 469 (*synth, cryst struct*)
Conradi, E. *et al*, *Chem. Ber.*, 1986, **119**, 2582 (*synth, cryst struct*)
Bohrer, R. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **558**, 119 (*synth, cryst struct*)

$Br_6U^{\ominus}$

Hexabromouranate(*V*)(1−) IC-002194
[44491-06-7]

$[UBr_6]^{\ominus}$ (O_h)

M 717.4 (ion)
Et_4N salt: [25630-17-5].
Moisture-sensitive dark red (black) cryst. Sol. $MeNO_2$, CH_2Cl_2. Ir ν_{UBr} 214 cm^{-1}.
Ph_4P salt: [115506-56-4].
Brown cryst. Also obt. as CCl_4 solvate.
Ph_4As salt: [25630-16-4].
Moisture-sensitive black cryst. Sol. $MeNO_2$, CH_2Cl_2. Ir ν_{UBr} 215 cm^{-1}.

Brown, D. *et al*, *J. Chem. Soc. A*, 1970, 476 (*synth, ir, uv-vis*)
Ryan, J.L., *J. Inorg. Nucl. Chem.*, 1971, **33**, 153 (*ir, synth, uv-vis*)
Inorg. Synth., 1974, **15**, 239 (*synth*)
Bohrer, R. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **558**, 119 (*synth, cryst struct*)

$Br_6V^{3\ominus}$

Hexabromovanadate(*III*)(3−) IC-002195
[36830-80-5]

$[VBr_6]^{3\ominus}$ (O_h)

M 530.3 (ion)
Li, di-Cs salt: [69208-00-0]. *Caesium lithium hexabromovanadate*(III) (Cs_2LiVBr_6)
Br_6Cs_2LiV M 803.1
Synth. by dissolving CsCl, Li_2CO_3 and V_2O_5 in 48% HBr. Has the bromo-Elpasolite struct.
Tris-pyridinium salt: [12105-50-9].
Synth. by reaction of VBr_3.3MeCN and [PyH]Br in $CHCl_3$. Orange-brown solid. Paramagnetic, μ_{eff} = 2.81μ_B.

Fowles, G.W.A. *et al*, *J. Chem. Soc. A*, 1967, 517 (*synth, magnetism*)
Meyer, G. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1476 (*synth, cryst struct, Cs_2Li salt*)

$Br_6W^{2\ominus}$

Hexabromotungstate(*IV*)(2−), 11Cl, 10Cl, 8Cl IC-002196
[20581-19-5]

$[WBr_6]^{2\ominus}$ (O_h)

M 663.2 (ion)
Di-K salt: [60950-21-2]. *Potassium hexabromotungstate*(IV)
Br_6K_2W M 741.4
Green cryst. solid.
Di-Rb salt: [61104-74-3]. *Rubidium hexabromotungstate*(IV)
Br_6Rb_2W M 834.2
Green cryst. solid.
Di-Cs salt: [29892-51-1]. *Caesium hexabromotungstate*(IV)
Br_6Cs_2W M 929.0
Green cryst. solid.

Kennedy, C.D. *et al*, *J. Chem. Soc.*, 1963, 3392 (*synth, props*)
Brown, T.L. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 3645 (*synth, nqr*)
Brown, T.L. *et al*, *J. Phys. Chem.*, 1970, **74**, 3572 (*nqr*)
Jenkins, H.D.B. *et al*, *J. Chem. Educ.*, 1979, **56**, 576 (*calcs*)
Burgess, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1143 (*thermochem*)

IC-002197

Br_6W

Tungsten(*VI*) bromide (WBr_6)

Tungsten hexabromide

[13701-86-5]

WBr_6 (O_h)

M 663.2

Molecular struct. Obt. by reaction of Br_2 with W or $W(CO)_6$. Dark blue solid. Readily hydrol. to tungstic acid.

Pascal, P., *Nouveau Traité de Chimie Minérale*, Masson, Paris, 1959, **XIV**, 821.

Willing, W. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 1425 (*struct*)

IC-002198

$Br_6Zr^{2\ominus}$

Hexabromozirconate(*IV*)(2 –), 1Cl

[33751-29-0]

$[ZrBr_6]^{2\ominus}$ (O_h)

M 570.6 (ion)

Di-K salt: [66169-91-3].

Br_6K_2Zr M 648.8

Synth. by heating KBr and $ZrBr_4$ in a sealed quartz tube at 550°.

Di-Cs salt: [36407-58-6].

Br_6Cs_2Zr M 836.4

Synth. from CsBr and $ZrBr_4$ in conc. HBr or by fusion. Widely used as a host lattice to study eg. luminescence of guest ions.

Bis-Et_4N salt: [23868-88-4].

Synth. by electrolytic oxidation of Zr in THF/Br_2 followed by addition of Et_4NBr. White solid.

Briadon, B.J. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 1969 (*uv*)

Van Bronswyk, W. *et al*, *Inorg. Chem.*, 1969, **8**, 1395 (*synth, ir, raman, Et_4N salt*)

Makhija, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1707 (*synth, thermochem, Cs,K salts*)

Flint, C.D. *et al*, *Inorg. Chem.*, 1981, **20**, 1768 (*use as host*)

Yoo, R.K. *et al*, *Chem. Phys.*, 1986, **108**, 317 (*use as host*)

IC-002199

$Br_7^{\ominus}$

Heptabromide(1 –)

[44606-76-0]

$[Br_7]^{\ominus}$

M 559.3 (ion)

Species formed electrochemically in Br_2 rich solns. Forms dark red salts. Dissociates in H_2O. Salts have high bromine vapour pressure.

Tetrabutylammonium salt: [38932-81-9].

Ralle, F. *et al*, *J. Electrochem. Soc.*, 1972, **119**, 1471 (*synth*)

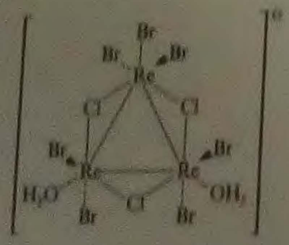
Eustace, D.J., *J. Electrochem. Soc.*, 1980, **127**, 528.

IC-002200

$Br_7Cl_3H_4O_2Re_3^{\ominus}$

Disquaheptabromotrichlorotrirhenate(*III*)(1 –), 8Cl

Trichloroheptabromodiaquatrirhenate(III)(*1 –*)



M 1260.3 (ion)

Cs salt: [24778-65-2].

Synth. from CsCl, $ReBr_3$ and HBr aq. Red cryst.

Hickford, J.H. *et al*, *J. Chem. Soc. A*, 1967, 113 (*synth, props*)

Elder, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 731 (*cryst struct*)

IC-002201

$Br_7Ga_2^{\ominus}$

μ-Bromohexabromodigallate(1 –)

[65643-76-7]

$[Br_3GaBrGaBr_3]^{\ominus}$

M 698.7 (ion)

Na salt: [75094-42-7].

Br_7Ga_2Na M 721.7

Synth. from NaBr and $GaBr_3$ melt. Colourless moisture-sensitive cryst.

Rb salt: [52582-11-3].

Br_7Ga_2Rb M 784.2

Synth. from RbBr and $GaBr_3$ melt. Colourless moisture-sensitive cryst. Mp 125°.

Cs salt: [52724-44-4].

Br_7CsGa_2 M 831.6

From CsBr and $GaBr_3$ melt. Colourless moisture-sensitive cryst. Mp 170°.

Mascherpa-Corral, D. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 1912 (*phase diagram*)

Dudareva, A.G. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 874 (*phase diagram*)

Mascherpa-Corral, D. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1977, **74**, 1077 (*dta, ir, raman*)

Fichter, W. *et al*, *Z. Naturforsch., B*, 1980, **35**, 170 (*nqr*)

IC-002202

Br_7In_4

Indium bromide (In_4Br_7)

Indium(1 +) hexabromoindate(3 –) tetrabromoindate(1 –) (3:1:2)

[12234-26-3]

$5In^{\oplus}\ 2[InBr_4]^{\ominus}[InBr_6]^{3\ominus}$

M 1018.6

Light green moisture-sensitive solid (melt).

[53184-02-4]

Walter, P.H.L. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **19**, 223 (*synth, struct*)

Moraweitz, W. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **316**, 220 (*synth*)

Davies, J.E. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 805 (*raman*)

IC-002203

Br_7In_5

Indium bromide (In_5Br_7)

Indium(1 +) bromide hexabromodiindate(2 –) (3:1:1).

Triindium(1 +) bromide hexabromoindate

[53199-64-7]

$3In^{\oplus}[In_2Br_6]^{2\ominus}Br^{\ominus}$

M 1133.4

May be identical with compd. earlier designated as In_2Br_3. Yellow platelets, becomes red below Mp. Mp 234°.

Walter, P.H.L. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **19**, 223 (*phase diagram*)

Moraweitz, W. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **316**, 220 (*synth*)

Davies, J.E. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 805 (*raman*)

IC-002204

Br_7NP_2

(Tetrabromophosphoranyl)phosphorimidic tribromide, 9CI

Tribromophosphorimidic tribromidato bromide

[58477-46-6]

$Br_3P{=}NPBr_4$ or $[Br_3P{=}NPBr_3]^{\oplus}\ Br^{\ominus}$

M 635.2

May possess ionic struct. Synth. from $PBr_3 + Br_2 + NH_4Br$. Orange solid; dec. at 125°. Forms yellow or red cryst. adducts with Br_2.

John, K. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **22**, 199.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 536 (*rev, bibl*)

Walsh, E.J. *et al*, *Inorg. Chim. Acta*, 1976, **16**, L9 (*synth*)

IC-002205

Br_7P

Tetrabromophosphonium tribromide

Tetrabromophosphorus(1 +) tribromide.

Heptabromophosphorus. Phosphorus bromide (PBr_7)

[12280-22-7]

$[PBr_4^{\oplus}]Br_3^{\ominus}$

M 590.3

Orthorhombic. Tetrahedral cation with P—Br 217 pm, and linear anion with P-Br 2.91, 2.39 pm. From $PBr_3 + Br_2$ with rapid cooling. Red cryst. V. hygroscopic and easily loses Br.

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 504 (*rev, bibl*)

Gorenbein, E.Y. *et al*, *Zh. Neorg. Khim.*, 1966, **11**, 2230; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1966, **11**, 1195 (*synth*)

Breneman, G.L. *et al*, *Acta Crystallogr.*, 1967, **23**, 467 (*synth, cryst struct*)

Breneman, G.L. *et al*, *J. Phys. Chem.*, 1967, **71**, 3684 (*nqr*)

Dhamelincourt, P. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 2470 (*raman*)

Gabes, W. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1971, **90**, 157 (*synth, raman*)

IC-002206

$Br_8Cl_4Mo_6$

Molybdenum bromide chloride ($Mo_6Br_8Cl_4$)

Octabromohexamolybdenum tetrachloride. Octa-μ_3-bromotetrachlorohexamolybdenum

[11057-07-1]

$Mo_6Br_8Cl_4$

M 1356.6

Presumed to contain clusters of Mo_6 octahedra. Prepd. by addition of HCl to alk. $MoBr_2$ solns.

Sheldon, J.C., *J. Chem. Soc.*, 1962, 410 (*synth*)

IC-002207

$Br_8Cl_4W_6$

Octabromotetrachlorohexatungsten

Tungsten bromide chloride ($W_6Br_8Cl_4$)

[48169-39-7]

$(W_6Br_8)Cl_4$

M 1884.1

Prepd. from $(W_6Br_8)Br_4$ by halide exchange with HCl. Cryst.

[27615-65-2]

Hogue, R.D. *et al*, *Inorg. Chem.*, 1970, **9**, 1354 (*synth, ir*)

IC-002208

$Br_8F_4W_6$

Octabromotetrafluorohexatungsten

Tungsten bromide fluoride ($W_6Br_8F_4$)

[27815-66-3]

$(W_6Br_8)F_4$

M 1818.3

Prepd. from $(W_6Br_8)Br_4$ by halide exchange. Cryst.

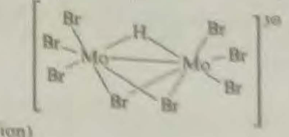
Hogue, R.D. *et al*, *Inorg. Chem.*, 1970, **9**, 1354 (*synth, ir*)

IC-002209

$Br_8HMo_2^{3\ominus}$

Di-μ-bromohexabromo-μ-hydrodimolybdate(*III*)(3 –)

[86253-64-3]



M 832.1 (ion)

Diamagnetic.

Tri-Cs salt: [57719-38-7].

$Br_8Cs_3HMo_2$ M 1230.8

Synth. from CsBr and $Mo_2(OAc)_4$ in conc. HBr

Reddish-yellow plate-like cryst. Originally incorrectly formulated as $Cs_3[Mo_2Br_8]$.

Bis-Me_4N, $H_3O_3^{\oplus}$ salt: [98117-84-1]. *Diaqua-μ_3-oxotrihydrogen(1 +) bis(tetramethylammonium) salt*

Synth. from $Mo_2(OAc)_4$ and $[Me_4N]Br$ in 8*M* aq. HBr at 70°. Dark yellow-brown cryst.

Cotton, F.A. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 1515 (*synth, cryst struct*)

Cotton, F.A. *et al*, *Inorg. Chem.*, 1976, **15**, 522 (*ir, reformulation*)

Bino, A., *Inorg. Chim. Acta*, 1985, **101**, L7 (*cryst struct, synth*)

IC-002210

$Br_8H_4Mo_6O_4$

Molybdenum bromide hydroxide ($Mo_6Br_8(OH)_4$)

Octabromohexamolybdenum tetrahydroxide

$Mo_6Br_8(OH)_4$

M 1282.9

A Mo_6 octahedral cluster compd. Isol. from alk. solns. of $MoBr_2$. Dark-brown amorphous powder. Forms a tetradecahydrate (yellow cryst.), which is isomorphous with $[(Mo_6Cl_8)(OH)_4(H_2O)_2].12H_2O$.

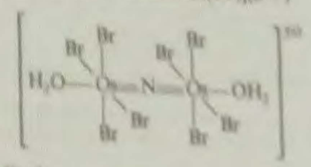
Sheldon, J.C., *J. Chem. Soc.*, 1962, 410 (*synth*)

IC-002211

$Br_8H_4NO_3Os_2^{3\ominus}$

Diaquaoctabromo-μ-nitridodiosmate(*IV*)(3 –)

μ-Nitridobis[aquatetrabromoosmate(IV)](3 –)



M 1069.6 (ion)

Tri-Cs salt: [27119-63-7].

Obt. by reaction of $(NH_4)_2[OsBr_6]$ with Br_2 at 450° in $Y_{Os-N-Os}$ 1070 cm^{-1}.

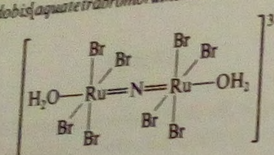
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1970, 1117 (*synth, ir*)

IC-002212

$Br_6H_4NO_2Ru_2^{3\ominus}$

Diaquaoctabromo-μ-nitridodiruthenate(3−), 9CI

μ-Nitridobis[aquatetrabromoruthenate(IV)]



M 891.4 (ion)

All salts are diamagnetic. Sol. H_2O, aq. HBr. The halide ions are very labile.

Tri-K salt: [21869-69-2].

$Br_6H_4K_3NO_2Ru_2$ M 1008.7

Prepd. by treating $[Ru_2NCl_8(OH_2)_2]^{3\ominus}$ with aq. KOH, followed by aq. HBr. Black cryst. Ir ν_{Ru_2N} 1050; ν_{RuBr} 254, 252 cm^{-1}.

[42735-86-4]

Cleare, M.J. *et al, J. Chem. Soc. A*, 1970, 1117 (*synth, str*)
Mattes, R. *et al, Z. Naturforsch., B*, 1975, **30**, 210 (*ir, raman*)

IC-002213

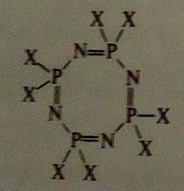
$Br_8N_4P_4$

2,2,4,4,6,6,8,8-Octabromo-2,2,4,4,6,6,8,8-octahydro-1,3,5,7,2,4,6,8-tetrazatetraphosphocine, 9CI, 8CI

Octabromocyclotetraphosphonitrile.

Octabromocyclotetraphosphazene. Tetrameric phosphorus nitride dibromide. 2,2,4,4,6,6,8,8-Octabromo-2λ⁵,4λ⁵,6λ⁵,8λ⁵-cyclotetraphosphaza-1,3,5,7-tetraene

[14621-11-5]



X = Br

M 819.1

Conformation intermed. between boat and saddle. Interatomic solid state distances: P—N, 157.5, P—Br, 217.1 pm (solid state); angles: PNP 131.0°, NPN 120.1°, BrPBr 103.9°. Synth. from NH_4Br + PBr_5. Tetragonal cryst. (heptane or pet. ether). Mp 202°. When heated in sealed tube at 220°, or subjected to γ irradiation at 80-150°, yields homopolymer.

Homopolymer: Tough, rubbery elastomer between −15 to 270°. Mp ~270°.

Inorg. Synth., 1963, **7**, 76 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 565 (*rev, bibl*)
Coxon, G.E. *et al, J. Chem. Soc. A*, 1967, 1568 (*ms*)
Manley, T.R. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 149 (*ir, raman*)
Lakatos, B. *et al, Acta Chim. (Budapest)*, 1969, **60**, 309 (*us, struct*)
Zoer, H. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 252 (*cryst struct*)
Allcock, H.R., *Phosphorus-Nitrogen Compounds*, Academic Press, London, 1972.
Horn, H.G. *et al, Makromol. Chem.*, 1975, **176**, 1359 (*P-31 nmr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 556 (*synth*)
Novobilsky, V., *Z. Anorg. Allg. Chem.*, 1976, **427**, 189 (*tlc*)
Thomas, B. *et al, Phosphorus Sulfur*, 1981, **10**, 375 (*N-15 nmr*)
Sridharan, K.R. *et al, Polyhedron*, 1983, **2**, 427 (*ngr*)

Br_8Nb_3

Niobium bromide (Nb_3Br_8), 11CI

Triniobium octabromide

IC-002214

[12049-24-0]

Nb_3Br_8

M 917.9

Struct. probably analogous to Niobium chloride (Nb_3Cl_8), IC-017416. Synth. by thermal dec. of $NbBr_4$ or by Zn reduction of $NbBr_5$ at 550-600°. Black, moisture-stable solid.

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1961, **311**, 139 (*synth*)
Berdonosov, S.S. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 1525 (*synth, struct*)
Simon, A. *et al, J. Less-Common Met.*, 1966, **11**, 31 (*synth*)
Fleming, P.B. *et al, Inorg. Chem.*, 1967, **6**, 1 (*synth, reactions*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1446 (*synth*)

$Br_8O_2Si_3$

Octabromotrisiloxane, 9CI

IC-002215

$Br_3SiOSiBr_2OSiBr_3$

M 755.4

Synth. from elements. Colourless liq. freezing in ice to colourless solid. Mp 17.5°. Bp_{12} 159°.

Schumb, W.C. *et al, J. Am. Chem. Soc.*, 1937, **59**, 261 (*synth*)

$Br_8O_4Si_4$

Octabromocyclotetrasiloxane

IC-002216

M 815.5

Product of oxidation of $SiBr_4$. Mp 123.5°. Bp 297°, Bp_7 155°.

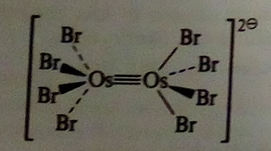
Rheinbolt, H. *et al, Justus Liebigs Ann. Chem.*, 1935, **517**, 197 (*synth*)
Schumb, W.C. *et al, J. Am. Chem. Soc.*, 1937, **59**, 261 (*synth*)

$Br_8Os_2^{2\ominus}$

IC-002217

Octabromodiosmate(*III*)(2−)

[97523-25-6]



M 1019.6 (ion)

Ligands staggered about Os—Os. Ion obt. by reaction of dry $Os_2(OAc)_4Cl_2$ with HBr.

Bis-tetrabutylammonium salt: [97523-38-1].

Green cryst. (CH_2Cl_2).

Fanwick, P.E. *et al, J. Am. Chem. Soc.*, 1985, **107**, 5009 (*synth, us*)
Fanwick, P.E. *et al, Inorg. Chem.*, 1986, **25**, 4547 (*synth*)
Pradyot, A.A. *et al, J. Am. Chem. Soc.*, 1986, **108**, 4851 (*cryst struct, synth*)

IC-002218

$Br_8Re_2^{2\ominus}$

Octabromodirhenate(*III*)(2−), 9CI

[19584-25-9]

$[Br_4ReReBr_4]^{2\ominus}$

M 1011.6 (ion)

Has eclipsed configuration with Re—Re 222.8 pm (Cs salt).

Di-Cs salt: [29032-77-7].

$Br_8Cs_2Re_2$ M 1277.4

Synth. (i) from $KReO_4$, CsBr and H_3PO_2 in 48% HBr. (ii) By halogen exchange from $Cs_2Re_2Cl_8$. Olive green cryst.

Bis-tetrabutylammonium salt: [14049-60-6].

Obt. from $Re_2(O_2CPh)_4Cl_2$, Bu_4NBr and HBr in MeOH. Olive green cryst.

Cotton, F.A. *et al, Inorg. Chem.*, 1970, **9**, 2143 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1629, 1630 (*synth*)
Glicksman, H.D. *et al, Inorg. Chem.*, 1978, **17**, 3197.
Cotton, F.A. *et al, Multiple Bonds Between Metal Atoms*, Wiley, New York, 1982, 42 (*synth, struct, props*)

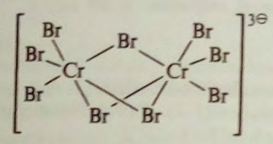
IC-002219

$Br_9Cr_2^{3\ominus}$

Tri-μ-bromohexabromodichromate(*III*)(3−), 11CI

Tri-μ-bromobis[tribromochromate(III)]

[45976-44-1]



M 823.1 (ion)

Tri-Cs salt: [24354-98-1].

$Br_9Cr_2Cs_3$ M 1221.8

Synth. from melt using CsBr and $CrBr_3$ at 790°. Green cryst.

Saillant, R. *et al, Inorg. Chem.*, 1971, **10**, 1453 (*cryst struct*)
Leuenberger, B. *et al, J. Solid State Chem.*, 1986, **64**, 90 (*struct, synth, magnetism*)

IC-002220

Br_9In_7

Indium bromide (In_7Br_9)

Indium(1+) bromide hexabromoindate(3−) (6:3:1).

Hexaindium(1+) tribromide hexabromoindate

[39310-66-2]

$6In^{\oplus}[InBr_6]^{3\ominus}3Br^{\ominus}$

M 1522.8

Obt. as intermediate in complex reactions between InBr and alkyl bromides. Yellow solid. Dec. > 200°.

[41099-58-5]

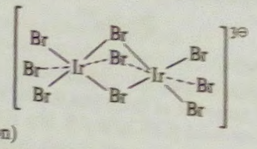
Waterworth, L.G. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 237 (*synth, raman*)
Davies, J.E. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 805 (*synth, raman*)

$Br_9Ir_2^{3\ominus}$

Tri-μ-bromohexabromodiiridate(*III*)(3−), 11CI

Nonabromodiiridate(III)(3−)

IC-002221



M 1103.5 (ion)

Tri-Rb salt: [86638-22-4].

$Br_9Ir_2Rb_3$ M 1359.9

Brown solid.

Tri-Cs salt: [86638-23-5].

$Br_9Cs_3Ir_2$ M 1502.2

Fergusson, J.E. *et al, Aust. J. Chem.*, 1983, **36**, 863 (*synth, powder struct*)

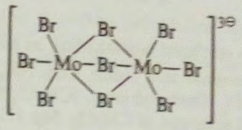
$Br_9Mo_2^{3\ominus}$

Tri-μ-bromohexabromodimolybdate(*III*)(3−), 9CI

Nonabromodimolybdate(III)(3−)

IC-002222

[45976-45-2]



M 911.0 (ion)

Cofacial bioctahedral arrangement around each Mo; Mo—Mo 257-278 pm. $Mo_2Cl_9^{3\ominus}$ and $Mo_2I_9^{3\ominus}$ analogues are also known.

Tri-K salt: [111533-06-3].

$Br_9K_3Mo_2$ M 1028.3

Cryst. Mo—Mo 257 pm.

Tri-Cs: [29013-06-7].

$Br_9Cs_3Mo_2$ M 1309.7

Synth. by reaction between $MoBr_3$ and CsBr at 770°. Air stable deep red cryst. (by subl.). Insol. H_2O. Subl. 770°. Mo—Mo 282 pm; μ_{eff} = 0.8μ_B (293K); temp. dependent.

Tri-rubidium salt: [111533-07-4].

$Br_9Mo_2Rb_3$ M 1167.4

Cryst. Mo—Mo 273 pm.

Saillant, R. *et al, Inorg. Chem.*, 1969, **8**, 1226; 1971, **10**, 1453 (*deriv*)
Zelentsov, V.V. *et al, Zh. Neorg. Khim.*, 1973, **18**, 2790 (*deriv*)
Bino, A. *et al, J. Am. Chem. Soc.*, 1980, **102**, 4277 (*use*)
Spitsin, V.I. *et al, Zh. Neorg. Khim.*, 1985, **30**, 2554 (*deriv*)
Stranger, R. *et al, J. Solid State Chem.*, 1987, **69**, 162 (*deriv*)
Stranger, R. *et al, Inorg. Chem.*, 1989, **28**, 1271 (*deriv*)

$Br_9O_4Pb_8Tl$

IC-002223

Lead thallium bromide oxide ($Pb_8TlBr_9O_4$)

[84285-89-2]

$TlPb_8O_4Br_9$

M 2645.1

Consists of isolated $Pb_8O_4^{18\ominus}$ units with 7- and 8-coord. Pb and 8-coordinate Tl. Cryst.

Keller, H.L., *Z. Anorg. Allg. Chem.*, 1982, **491**, 191 (*synth, cryst struct*)

IC-002224

$Br_9Re_2^{2\ominus}$

Nonabromodirhenate(*III,IV*)(2−)

Tri-μ-bromohexabromodirhenate(2−)

$[Re_2Br_9]^{2\ominus}$

M 1091.5 (ion)

Bis-tetrabutylammonium salt: [19584-23-7].
Synth. by reduction of $[Bu_4N]Re_2Br_9$ by Fe in Me_2CO. Rusty-brown solid ($CHCl_3/Et_2O$). Mp 122° dec.

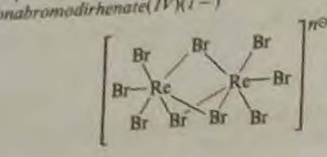
Bonati, F. *et al, Inorg. Chem.*, 1967, **6**, 1353 (*synth, ir, uv, props*)

IC-002225

$Br_9Re_2^{\ominus}$

Tri-μ-bromohexabromodirhenate(1−)

Nonabromodirhenate(IV)(1−)



$n = 1$

M 1091.5 (ion)
Believed to be confacial bioctahedral, as shown.
Tetrabutylammonium salt: Synth. from $(Bu_4N)_4Re_2Br_8$ and Br_2 in CH_2Cl_2. Dark red cryst. ($CH_2Cl_2/CHCl_3$). More sol. than Cl analogue in CH_2Cl_2. Mp 171° dec.

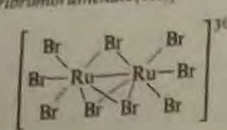
Bonati, F. *et al, Inorg. Chem.*, 1967, **6**, 1353 (*synth, ir, uv, props*)

IC-002226

$Br_9Ru_2^{3\ominus}$

Tri-μ-bromohexabromodiruthenate(*III*)(3−), 10Cl

Nonabromodiruthenate(III). *μ-Tribromobis[tribromoruthenate*(III)]



M 921.2 (ion)
Essentially an ideal confacial bioctahedron, containing a significant metal-metal bond. Formed by dissolving $RuBr_3.xH_2O$ in HBr in the presence of EtOH. Aq. HBr solns. are readily oxidized to $[RuBr_6]^{2\ominus}$ in air. V. sol. aq. HBr. Salts previously reported as containing $[Ru_2OBr_{10}]^{4\ominus}$ are now known to contain $[Ru_2Br_9]^{3\ominus}$, as are salts previously reported to contain $[Ru(OH_2)Br_5]^{2\ominus}$.

Tri-K salt: [66115-10-4].
$Br_9K_3Ru_2$ M 1038.5
Usually contaminated with minor levels of KBr. Purple-black cryst. (hexagonal). ν_{RuBr}, 267, 244 cm^{-1}.

Tri-Rb salt: [66115-11-5].
$Br_9Rb_3Ru_2$ M 1177.6
Purple-black cryst. Ir ν_{RuBr}, 260, 240 cm^{-1}

Tri-Cs salt: [66162-09-2].
$Br_9Cs_3Ru_2$ M 1319.9
Purple-black cryst. Ir ν_{RuBr}, 258, 236 cm^{-1}; μ_{eff} = 1.01μ_B/Ru atom; Ru—Ru 286 pm.

Tris-tetrabutylammonium salt: Purple cryst. Sol. CH_2Cl_2. Ir ν_{RuBr}, 262, 229 cm^{-1}; μ_{eff} = 1.19μ_B/Ru atom.

Benzyltriphenylphosphonium salt: Purple cryst.

1-Ethyl-3-methylimidazolium salt: Purple cryst. Ir ν_{RuBr}, 254, 228 cm^{-1}; Ru—Ru 288, Ru—Br_{term} 251.2, Ru—Br_{br} 250.8 pm.

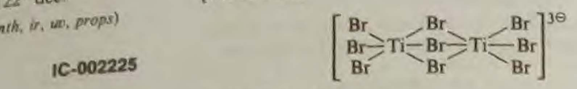
Fergusson, J.E. *et al, Aust. J. Chem.*, 1978, **31**, 497 (*synth, struct, ir*)
Coombe, V.T. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2307 (*synth, magnetism, electrochem, uv*)
Appleby, D. *et al, J. Chem. Soc., Dalton Trans.*, 1990, 1879 (*synth, cryst struct, uv, ir, electrochem, theory*)

IC-002227

$Br_9Ti_2^{3\ominus}$

Tri-μ-bromohexabromodititanate(*III*)(3−)

[90526-96-8]



M 814.8 (ion)
Contains octahedral Ti.
Tri-Rb salt: [12260-35-4]. *Rubidium nonabromodititanate*(III). *Trirubidium nonabromodititanate(3−). Rubidium titanium bromide* ($Rb_3Ti_2Br_9$)
$Br_9Rb_3Ti_2$ M 1071.2
Orange solid. Mp 647°. Antiferromagnetic, μ_{eff} = 1.34μ_B (300K), 0.71μ_B (80K).

Shchukarev, I.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1963, **8**, 1006 (*phase diagrams, Cs and Rb systems*)
Shchukarev, I.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 980 (*synth, enthalpy of form*)
Leuenberger, B. *et al, Chem. Phys. Lett.*, 1986, **126**, 255 (*synth, neutron scattering, magnetism, ir, Rb salt*)

IC-002228

$Br_9Tl_2^{3\ominus}$

Tri-μ-bromohexabromodithallate(3−)

Nonabromodithallate(3−). Tetrabromothallate(1−) pentabromothallate(2−), 12Cl

$[Tl_2Br_9]^{3\ominus}$

M 1127.9 (ion)

▷ Toxic.

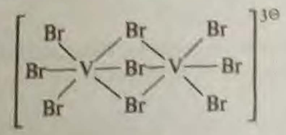
Tri-Cs salt: [79060-94-9].
Synth. from CsBr/TlBr in 3:2 mol. ratio in a closed system at 400° or by heating aq. soln. α→β phase transition occurs at 170°. The β-form is isostructural with $Cs_3Bi_2Br_9$; the α-form contains chains of $TlBr_6$ octahedra and isolated $TlBr_4$ tetrahedra.

Zimmermann, K. *et al, Z. Naturforsch., B*, 1987, **42**, 818 (*synth, struct, raman*)

IC-002229

$Br_9V_2^{3\ominus}$

Tri-μ-bromohexabromodivanadate(*III*)(3−), 11Cl



M 821.0 (ion)
Face-shared octahedra.
Tri-Rb salt: [102682-48-4]. *Rubidium vanadium bromide* ($Rb_3V_2Br_9$)
$Br_9Rb_3V_2$ M 1077.4
Synth. from a melt of RbBr and VBr_3 at 700°. Mag. susc. shows a max. at 12K; J = 5.2 cm^{-1}. Neutron scattering does not show magnetic ordering.

Leuenberger, B. *et al, Inorg. Chem.*, 1986, **25**, 2930 (*synth, neutron scattering, mcd, magnetism*)

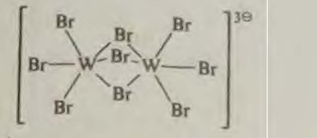
IC-002230

$Br_9W_2^{3\ominus}$

Tri-μ-bromohexabromoditungstate(3−), 9Cl

Nonabromoditungstate(3−)

[72428-80-9]



M 1086.8 (ion)
Prepd. from $[W_2Cl_9]^{3\ominus}$ and $Br^{\ominus}$.
Tri-K salt:
$Br_9K_3W_2$ M 1204.1
Brown, hexagonal plates.

[21732-21-8, 72332-25-3]

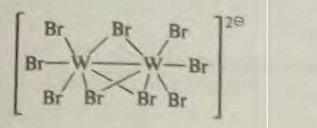
Hayden, J.L. *et al, J. Am. Chem. Soc.*, 1968, **90**, 5291 (*synth, uv*)

IC-002231

$Br_9W_2^{2\ominus}$

Tri-μ-bromohexabromoditungstate(2−), 10Cl, 9Cl

[60267-85-8]



M 1086.8 (ion)
Confacial bioctahedral struct., mixed valence compd. with W—W bond order 2.5; W—W 260.1 pm. μ_{eff} = 1.72μ_B per formula unit (77-300K).
Bis-tetrapropylammonium salt: [60318-96-9].
Black cryst. (MeCN) (dark green when crushed).

McCarley, R.E. *et al, Adv. Chem. Ser.*, 1976, **150**, 318.
Templeton, J.L. *et al, Inorg. Chem.*, 1977, **16**, 3320 (*cryst struct*)
Trogler, W.C., *Inorg. Chem.*, 1980, **19**, 697.

IC-002232

$Br_{10}NNb_2^{3\ominus}$

Decabromo-μ-nitridodiniobate(*V*)(3−), 11Cl

$[Br_5NbNNbBr_5]^{3\ominus}$ (D_{4h})

M 998.8 (ion)
Bioctahedral with linear Nb—N—Nb grouping.
Tri-NH_4 salt: [103111-12-2].
Synth. from $NbBr_5$ and $[NH_4]Br$. Cryst.

Hoerner, M. *et al, Z. Naturforsch., B*, 1986, **41**, 423 (*synth, cryst struct*)

IC-002233

$Br_{10}NTa_2^{3\ominus}$

Decabromo-μ-nitridoditantalate(*V*)(3−), 11Cl

(μ-Nitrido)bis(pentabromotantalate(V))

$[Br_5TaNTaBr_5]^{3\ominus}$

M 1174.9 (ion)
D_{4h}-symmetry with linear Ta-N-Ta bridge. Ta—N 185 pm. Corresp. iodo complex has the same struct.
Tri-NH_4 salt: [73820-91-4].
Synth. by heating $[NH_4]Br$ and $TaBr_5$ to 400° in a sealed glass ampoule. Greenish-yellow, moisture-sensitive solid.

Frank, K. *et al, Z. Naturforsch., B*, 1980, **35**, 300 (*synth, cryst struct*)
Hoerner, M. *et al, Z. Naturforsch., B*, 1986, **41**, 423 (*synth, cryst struct, iodo analogue*)

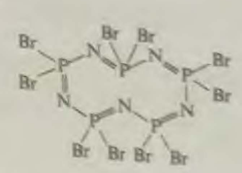
IC-002234

$Br_{10}N_5P_5$

2,2,4,4,6,6,8,8,10,10-Decabromo-2,2,4,4,6,6,8,8,10,10-decahydro-1,3,5,7,9,2,4,6,8,10-pentazapentaphosphecine, 9Cl, 8Cl

Decabromocyclopentaphosphanitrile. Decabromocyclopentaphosphazene. 2,2,4,4,6,6,8,8,10,10-Decabromo-2λ⁵,4λ⁵,6λ⁵,8λ⁵,10λ⁵-cyclopentaphosphazo-1,3,5,7,9-pentaene

[15763-08-3]



M 1023.9
Interatomic distances: P—N 157.1, P—Br 217.5 pm; angles: NPN 114.3, 120.5°, PNP 131.2, 136.6, 143.8°.
Synth. from PBr_5 + NH_4Br. Triclinic cryst. Mp 104.5°.

Coxon, G.E. *et al, J. Chem. Soc. A*, 1967, 1568 (*mi*)
Coxon, G.E. *et al, Spectrochim. Acta, Part A*, 1968, **24**, 2145 (*ir, raman*)
Hartsuiker, J.G. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1069 (*cryst struct*)
Novobilsky, V., *Z. Anorg. Allg. Chem.*, 1976, **427**, 189 (*dic*)

IC-002235

$Br_{10}OOs_2^{4\ominus}$

Decabromo-μ-oxodiosmate(*IV*)(4−)

μ-Oxobis[pentabromoosmate(IV)](4−)

[48063-44-1]

$[Br_5Os—O—OsBr_5]^{4\ominus}$

M 1195.4 (ion)
Previously thought to be $[OsBr_5OH]^{2\ominus}$. Linear Os—O—Os.

Tetra-Cs salt: [40530-84-5].
Tetrakis-$MeNH_3$ salt: Bright brown cryst. Sol. EtOH, H_2O.

[31495-97-3]

Griffith, W.P., *J. Chem. Soc. A*, 1966, 472; 1969, 211 (*ir, synth*)
Hanuza, J. *et al, Acta Phys. Pol. A*, 1970, **38**, 563; 1972, **42**, 537 (*ir, theory*)

IC-002236

$Br_{10}ORu_2^{4\ominus}$

Decabromo-μ-oxodiruthenate(4−), 9Cl

μ-Oxobis[pentabromoruthenate(IV)]

[48063-50-9]

$[Ru_2OBr_{10}]^{4\ominus}$

M 1017.1 (ion)
Non-existent sp. Despite many claims as to the prepn. and characterization of this species, it is now known not to exist (as yet); salts claimed in the literature to contain $[Ru_2OBr_{10}]^{4\ominus}$ actually contain $[Ru_2Br_9]^{3\ominus}$.

San Filippo, J. *et al, Inorg. Chem.*, 1976, **15**, 2809; 1977, **16**, 1066.
Appleby, D. *et al, J. Chem. Soc., Dalton Trans.*, 1990, 1879.

IC-002237

$Br_{10}O_4Pb_9$

Lead bromide oxide ($Pb_9Br_{10}O_4$)

Basic lead bromide

[85249-97-4]

$Pb_9O_4Br_{10}$

M 2727.8
Struct. contains $[Pb_6O_4]^{2\oplus}$ clusters. Cryst.
Keller, H.L., *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 324 (*synth, cryst struct*)

IC-002238

$Br_{10}Si_4$
Decabromotetrasilane, 9CI
[81626-34-8]

$Br_3SiSiBr_2SiBr_2SiBr_3$

M 911.3
Synth. by cleavage of octaphenylcyclotetrasilane with Br_2 followed by reaction with $HBr/AlBr_3$. Mp 82-84°.
Hassler, K. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **488**, 27 (*synth, ir, raman, Si-29 nmr*)

IC-002239

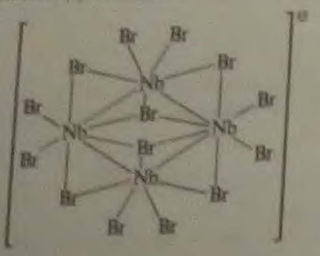
$Br_{11}Hg_3^{\ominus}$
Octa-μ-bromotribromopentamercurate(1−)
Undecabromopentamercurate(1−)

$[Hg_3Br_{11}]^{\ominus}$

M 1881.8 (ion)
Two different mercury environments: Hg(1) has 2 short Hg—Br and 4 long Hg—Br contacts, Hg(2) has 2 short Hg—Br and 5 long Hg—Br contacts.
K salt: [73912-79-5].
$Br_{11}Hg_3K$ M 1920.9
Cryst.
Tl(I) salt: [12049-27-3]. *Mercury thallium bromide* (Hg_3TlBr_{11})
$Br_{11}Hg_3Tl$ M 2086.2
Cryst. Dec. at 210°.
NH_4 salt: [73907-59-2].
Cryst.
Huart, J., *Bull. Soc. Fr. Mineral. Cristallogr.*, 1966, **89**, 23 (*thermal anal*)
Brodersen, K. *et al*, *Z. Naturforsch., B*, 1980, **35**, 253 (*synth, cryst struct*)

IC-002240

$Br_{11}Nb_4^{\ominus}$
Undecabromotetraniobate(1−)
Tetra-μ-bromodi-μ$_3$-bromopentabromotetraniobate(1−), 10CI

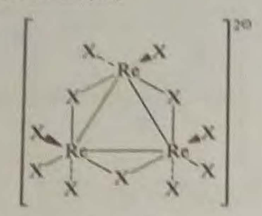


core cluster

M 1250.5 (ion)
Planar arrangement of 4 Nb, bridging Br on each edge and Br bridging 3 Nb. Each Nb is octahedral. Stoichiometry attained by extensive bridging between clusters.
Cs salt:
$Br_{11}CsNb_4$ M 1383.4
Synth. by heating CsCl, Nb_3Cl_8 and Nb in a sealed tube at 730/700°. Solid.
Broll, A. *et al*, *Z. Anorg. Allg. Chem.*, 1969, **367**, 1 (*synth, cryst struct, ir*)

IC-002241

$Br_{11}Re_3^{2\ominus}$
Tri-μ-bromooctabromotrirhenate(*III*)(2−), 8CI
Undecabromotrirhenate(III)

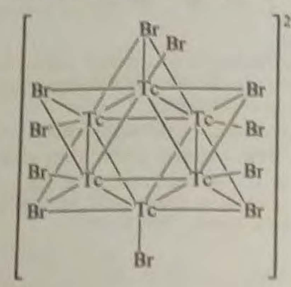


X = Br

M 1437.5 (ion)
Di-Cs salt:
$Br_{11}Cs_2Re_3$ M 1703.3
Synth. from CsBr and $ReBr_3$ in HBr aq. or in HBr/EtOH. Small black needle-shaped cryst.
Fergusson, J.E. *et al*, *Proc. Chem. Soc., London*, 1964, 189 (*synth, props*)
Elder, M. *et al*, *Inorg. Chem.*, 1966, **5**, 1763 (*cryst struct*)

IC-002242

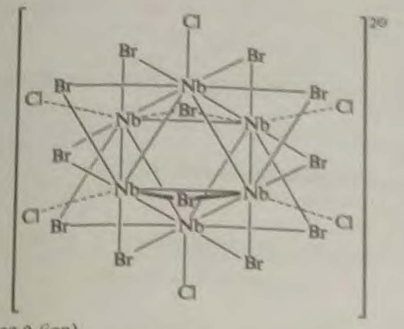
$Br_{11}Tc_6^{2\ominus}$
Undecabromohexatechnetate(2−)
Penta-μ$_3$-bromohexabromotechnetate(2−), 12CI



M 1472.3 (ion)
Octahedron of Tc atoms each with one terminal Br, and 5 Br over faces. This anion, with similar $[Tc_6Br_{12}]^{\ominus}$ and $[Tc_8Br_{13}]^{\ominus}$, is obt. by reaction of $HTcO_4$ or of H_2TcBr_6 with HBr.
Bis-tetrabutylammonium salt: [118674-37-6].
$\mu_{eff} \simeq 1.6\mu_B$.
Bis[$H_3O(OH_2)_3$]$^{\oplus}$ salt: [105857-22-5]. *Bis[triaqua-μ$_3$-oxotrihydrogen(1+)] undecabromohexatechnetate(2−)*
Reddish-black cryst. Sol. EtOH, polar org. solvs.
[106417-98-5]
Koz'min, P.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1982, **265**, 1420 (*analogues, cryst struct*)
Kryuchkov, S.V. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1986, **287**, 1400; **288**, 893 (*synth, ir, struct, analogues*)
Kryuchkov, S.V. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1986, **290**, 866 (*cryst struct, ir, magnetism*)
Spitsyn, V.I. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **563**, 136 (*synth, cryst struct, props, analogues*)
Kryuchkov, S.V. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **563**, 153 (*ir, esr, thermal stability, magnetism*)

IC-002243

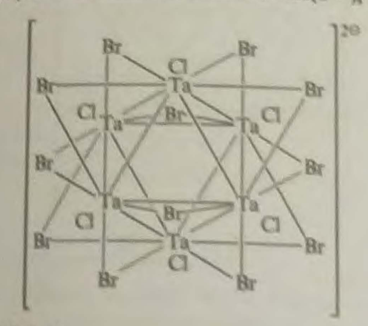
$Br_{12}Cl_6Nb_6^{2\ominus}$
Dodeca-μ-bromohexachlorohexaniobate(2−), 11CI
Hexaniobium dodecabromide hexachloride
[12514-58-8]



M 1729.0 (ion)
Bis-Et_4N salt: [12567-93-0].
Synth. by dissolving $[Nb_6Br_{12}]Br_2.8H_2O$ in EtOH saturated with HCl gas and oxidising with Cl_2, then adding $[Et_4N]Cl$. Black solid.
Bis-pyridinium salt: [11141-41-6].
Synth. by dissolving $[Nb_6Br_{12}]Br_2.8H_2O$ in EtOH, saturating with HCl, oxidising with H_2O_2 followed by Py in EtOH. Black solid. Transforms irreversibly into $[NbBr_6Cl_6]Br_6$ on heating.
Hughes, B.G. *et al*, *Inorg. Chem.*, 1970, **9**, 1343 (*synth*)
Fleming, P.B. *et al*, *Inorg. Chem.*, 1970, **9**, 1769 (*ir*)
Sprechelmeyer, B. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **386**, 15, 27 (*cryst struct, thermal conv*)

IC-002244

$Br_{12}Cl_6Ta_6^{2\ominus}$
Dodeca-μ-bromohexachlorohexatantalate(2−), 11CI



M 2257.2 (ion)
Presumed struct. shown.
Bis-Et_4N salt: [12555-94-1].
Synth. by Cl_2 oxidation of a soln. of $[Ta_6Br_{12}]^{2\oplus}$ in EtOH followed by $[Et_4N]Cl$. Deep red air-sensitive solid.
Bis-pyridinium salt: [11127-30-3].
Synth. by H_2O_2 oxidation of $Ta_6Br_{12}Cl_2$ in HCl/EtOH and addition of Py. At 200° converts exothermically to $[(Ta_6Br_6Cl_6)Br_6]^{2\ominus}$.
Hughes, B.G. *et al*, *Inorg. Chem.*, 1970, **9**, 1343 (*synth*)
Fleming, P.B. *et al*, *Inorg. Chem.*, 1970, **9**, 1769 (*ir*)
Sprekelmeyer, B. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **386**, 15 (*synth*)
Schaefer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **517**, 185 (*reaction*)

IC-002245

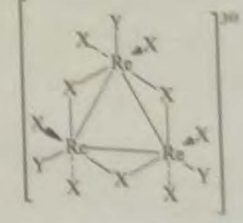
$Br_{12}Mo_6$
Molybdenum bromide (Mo_6Br_{12})
Octa-μ$_3$-bromotetrabromohexamolybdenum, 9CI. Molybdous bromide
[12234-30-9]

$[Mo_6Br_8]Br_4$

M 1534.4
The 6 Mo atoms are arranged in an octahedron with 8 Br-bridges between them. The other 4 Br atoms bridge between clusters. Prepd. from Mo + Br_2 at 600-700°, by fusing $MoCl_2$ with LiBr, or by disproportionation of $MoBr_3$. Yellowish-red amorphous powder. Hygroscopic. Infusible. Dissolves in warm strong bases to give $(Mo_6Br_8)(OH)_4.nH_2O$. Addition of conc. HCl or HI to an alk. soln. gives $(Mo_6Br_8)X_4$ (X = Cl, I). Insol. H_2O, EtOH; sol. boiling DMSO.
'Monomer': Molybdenum bromide ($MoBr_2$). Molybdenum dibromide
Br_2Mo M 255.7
Has no separate existence.
[9018-99-9, 13446-56-5, 43140-50-7]
Lindner, K. *et al*, *Z. Anorg. Allg. Chem.*, 1925, **142**, 180 (*synth*)
Sheldon, J.C. *et al*, *J. Chem. Soc.*, 1962, 410 (*synth*)
Schaefer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **353**, 281 (*synth, struct*)
Mattes, R., *Z. Anorg. Allg. Chem.*, 1968, **357**, 30 (*ir*)
Inorg. Synth., 1970, **12**, 170 (*synth*)
Oppermann, H., *Z. Anorg. Allg. Chem.*, 1973, **395**, 249 (*thermodyn*)
Best, S.A. *et al*, *Inorg. Chem.*, 1979, **18**, 484 (*pe*)

IC-002246

$Br_{12}Re_3^{3\ominus}$
Tri-μ-bromononabromotrirhenate(*III*)(3−), 8CI
Dodecabromotrirhenate(III)(3−)



X = Y = Br

M 1517.4 (ion)
Tri-Cs salt: [24669-21-4].
$Br_{12}Cs_3Re_3$ M 1916.1
Synth. from $ReBr_3$, CsBr and HBr aq. Red cryst.
Fergusson, J.E., *Coord. Chem. Rev.*, 1966, **1**, 459 (*props*)
Elder, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 731 (*synth, cryst struct*)

IC-002247

$Br_{12}Ru_5^{2\ominus}$
Ruthenium violet

$[Ru_5Br_{12}]^{2\ominus}$

M 1464.1 (ion)
The best (but probably incorrect) description of the chromophore present in ruthenium violet solns. Produced when aq. or alcoholic HBr soln. of $RuBr_3$ is reduced by H_2, Zn or Al. Analogues to Ruthenium blue. IC-017522. Valuable synthetic reagent. Violet-blue soln. Some poorly defined salts have been isol. Sol. H_2O, alcohols.

1,4-Xylylenebis(triphenylphosphonium)(2+) salt: Black solid.

Gall, H. *et al, Chem. Ber.*, 1926, **59**, 2856 (*synth*)
Joergensen, C.K., *Acta Chem. Scand.*, 1956, **10**, 518 (*synth*)
Rose, D. *et al, J. Chem. Soc. A*, 1970, 1791 (*synth, esr*)

IC-002248

$Br_{12}W_6$

Tungsten bromide (W_6Br_{12})

Octa-μ_3-bromotetrabromohexatungsten

[13470-10-5]

$(W_6Br_8)Br_4$

M 2061.9

Prepd. by disproportionation of WBr_4. Yellow-green cryst. Insol. H_2O.

'Monomer': Tungsten bromide (WBr_2). Tungsten dibromide
Br_2W M 343.6

[12234-31-0, 27615-64-1]

Emeleus, H.J. *et al, J. Chem. Soc.*, 1950, 2115 (*synth*)
McCarley, R.E. *et al, Inorg. Chem.*, 1964, **3**, 1232 (*synth*)
Mattes, R., *Z. Anorg. Allg. Chem.*, 1968, **357**, 30 (*ir*)

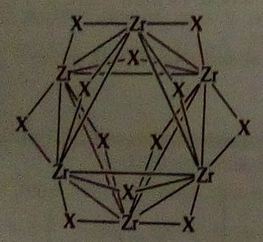
$Br_{12}Zr_6$

IC-002249

Zirconium bromide (Zr_6Br_{12})

Dodeca-μ-bromohexazirconium(II), 10CI

[75444-52-9]



X = Br

M 1506.1

Synth. by reaction of Zirconium bromide (ZrBr), IC-001759 and H_2 in temp. gradient. Cryst.

Imoto, H. *et al, Inorg. Chem.*, 1981, **20**, 145 (*synth, cryst struct*)

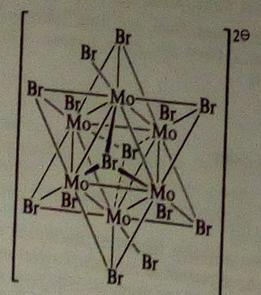
$Br_{14}Mo_6^{2\ominus}$

IC-002250

Octa-μ_3-bromohexabromohexamolybdate(2−), 9CI

Tetradecabromohexamolybdate(2−)

[52906-24-8]



M 1694.2 (ion)

A Mo_6 octahedral cluster ion.

Di-Rb salt: Solid. Mp 219° dec.

Di-Cs salt:
$Br_{14}Cs_2Mo_6$ M 1960.1
Prepd. from $MoBr_2$ + CsBr in IBr at 50°. Solid. Mp 210° dec.

Sheldon, J.C., *J. Chem. Soc.*, 1962, 410 (*synth*)
Opalovskii, A.A. *et al, Dokl. Akad. Nauk SSSR*, 1967, **174**, 1109 (*synth*)
Cotton, F.A. *et al, Inorg. Chem.*, 1967, **6**, 11 (*ir*)
Best, S.A. *et al, Inorg. Chem.*, 1979, **18**, 484 (*pe*)
Zelverte, A. *et al, Spectrochim. Acta, Part A*, 1986, **42**, 837 (*ir, raman*)

$Br_{14}W_6^{2\ominus}$

IC-002251

Tetradecabromohexatungstate(*II*)(2−)

Octa-μ_3-bromohexabromohexatungstate(2−), 11CI

[88477-00-3]

As Tetradecabromohexatungstate(1−), IC-002252 with

$n = 2$, X = Y = Br

M 2221.7 (ion)

Interatomic distance: W—W 263.5 pm.

Bis-tetrabutylammonium salt: [96390-92-0].
Bis[bis(triphenylphosphine)iminium] salt: [101955-15-1]. Cryst.

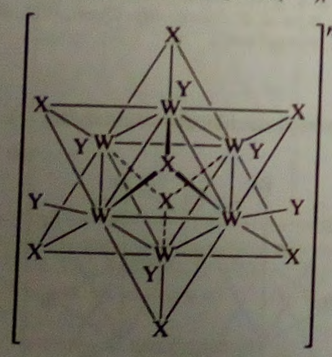
Hogue, R.D. *et al, Inorg. Chem.*, 1970, **9**, 1355 (*synth, ir*)
Zietlow, T.C. *et al, Inorg. Chem.*, 1986, **25**, 1351, 2195, 2198 (*cryst struct, synth, props*)

$Br_{14}W_6^{\ominus}$

IC-002252

Tetradecabromohexatungstate(1−)

Octa-μ_3-bromohexabromohexatungstate(1−), 11CI



$n = 1$, X = Y = Br

M 2221.7 (ion)

Interatomic distance: W—W 264.9 pm. Synth. by oxidation of Tetradecabromohexatungstate(*II*)(2−), IC-002251 with $NOPF_6$. Several relat. compds. with different halides also prepd.

Bis(triphenylphosphine)iminium salt: [101955-18-4]. Deep red cryst. (CH_2Cl_2/pet. ether).

Zietlow, T.C. *et al, Inorg. Chem.*, 1986, **25**, 2198 (*synth, cryst struct, uv, esr, magnetism*)

$Br_{15}Ta_6$

IC-002253

Tantalum bromide (Ta_6Br_{15}), 8CI

$[Ta_6Br_{12}]Br_3$

M 2284.2

Struct. comprises Ta_6Br_{12} octahedra with 3 Br occupying the remaining six positions randomly. Synth. by heating $TaBr_5$ + Ta. Paramagnetic, μ_{eff} = 2.17 (623K), 1.73 (222K), 1.34μ_B (77K).

Octahydrate:
$Br_{18}H_{16}O_8Ta_6$ M 2428.3
Synth. by oxidising $Ta_6Br_{14}.8H_2O$ with $KBrO_3$ in aq. soln.

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1965, **335**, 96 (*synth*)
Spreckelmeyer, B., *Z. Anorg. Allg. Chem.*, 1968, **358**, 147 (*synth, octahydrate, magnetism, uv-vis*)
Bauer, D. *et al, Z. Anorg. Allg. Chem.*, 1968, **361**, 259 (*cryst struct, magnetism*)
Converse, J.G. *et al, Inorg. Chem.*, 1970, **9**, 1361 (*synth, magnetism*)

$Br_{16}OsSn_5^{4\ominus}$

IC-002254

Bromopentakis(tribromostannyl)osmate(*II*)(4−)

Bromopentakis(tribromostannio)osmate(II)(4−)

[62137-12-6]

$[Os(SnBr_3)_5Br]^{4\ominus}$

M 2062.2 (ion)

Catalyst for hydrogenation of alkenes.

[62137-13-7]

Yurchenko, E.N. *et al, Koord. Khim.*, 1976, **2**, 1632 (*ir*)
Antonov, P.G. *et al, Koord. Khim.*, 1977, **3**, 757 (*use*)
Borunova, N.V. *et al, Zh. Obshch. Khim.*, 1980, **50**, 1862 (*use, synth*)
Yurchenko, E.N. *et al, Teor. Eksp. Khim.*, 1985, **21**, 194; *CA*, **103**, 95565 (*use*)

$Br_{16}Ta_6$

IC-002255

Tantalum bromide (Ta_6Br_{16}), 8CI

$[Ta_6Br_{12}]Br_4$

M 2364.1

Prob. contains Ta_6Br_{12} octahedra.

Heptahydrate:
$Br_{16}H_{14}O_7Ta_6$ M 2490.2
Synth. by oxidising $Ta_6Br_{14}.8H_2O$ or $Ta_6Br_{15}.8H_2O$ with $KBrO_3$ in aq. soln. Red-brown solid. Diamagnetic.

Spreckelmeyer, B., *Z. Anorg. Allg. Chem.*, 1968, **358**, 147 (*synth, magnetism, heptahydrate*)
Mattes, R., *Z. Anorg. Allg. Chem.*, 1969, **364**, 279 (*ir*)

$Br_{16}Ti_7$

IC-002256

Titanium bromide (Ti_7Br_{16}), 11CI

[69855-33-0]

Ti_7Br_{16}

M 1613.6

Triangular Ti(*II*) trimers (Ti_3Br_{13}) and octahedral Ti(*IV*) monomers are linked in a 3-D network. Synth. from Ti, Br_2 and Al_2Br_6 in a temp. gradient 350-250°. Black, moisture and oxygen sensitive solid. Antiferromagnetic, Néel temp. 18K (13.5K).

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1981, **474**, 135 (*synth, magnetism*)
Krebs, B. *et al, Z. Anorg. Allg. Chem.*, 1981, **474**, 149 (*cryst struct*)
Lueken, H. *et al, Z. Anorg. Allg. Chem.*, 1982, **490**, 64 (*magnetism*)

$Br_{16}W_6$

IC-002257

Tungsten bromide (W_6Br_{16})

Octa-μ_3-bromotetrabromo[tetrabromo(2−)]hexatungsten

W_6Br_{16}

M 2381.5

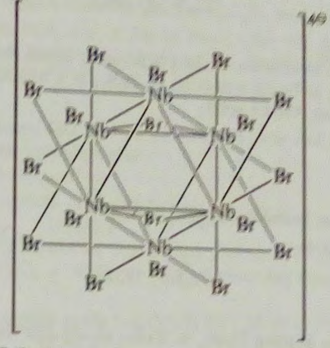
Prepd. by reaction of $(W_6Br_8)Br_4$ with Br_2. Black cryst.

Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1968, **357**, 273 (*synth*)
Siepmann, R. *et al, Z. Anorg. Allg. Chem.*, 1968, **357**, 289 (*cryst struct*)

$Br_{18}Nb_6^{4\ominus}$

IC-002258

Dodeca-μ-bromohexabromohexaniobate(4−), 11CI



M 1995.7 (ion)

Octahedron of Nb.

Tetra-K salt: [12765-98-9].
$Br_{18}K_4Nb_6$ M 2152.1
Synth. by heating $NbBr_5$, KBr and Nb in a sealed tube at 850°. Cryst. + $8H_2O$ (HBr aq.). The Na salt may be synthesised in the same way.

Parsons, J.A. *et al, Inorg. Nucl. Chem. Lett.*, 1972, **8**, 281 (*synth*)
Koknat, F.W. *et al, Inorg. Chem.*, 1974, **13**, 1699 (*synth*)
Ueno, F. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 308 (*cryst struct*)

$Br_{18}W_6$

IC-002259

Tungsten bromide (W_6Br_{18})

Octa-μ_3-bromodibromobis[tetrabromo(2−)]hexatungsten

[12049-33-1]

$[W_6Br_{12}]Br_6$

M 2541.3

Prepd. by reaction of $[W_6Br_8]Br_4$ with bromine. Black microcryst. powder.

'Monomer': Tungsten(III) bromide. Tungsten tribromide
Br_3W M 423.5

[15163-24-3]

Siepmann, R., *Naturwissenschaften*, 1965, **52**, 344 (*synth*)
Schaefer, H. *et al, Z. Anorg. Allg. Chem.*, 1968, **357**, 273 (*synth*)
Lange, U. *et al, J. Less-Common Met.*, 1970, **21**, 472 (*synth, cryst struct*)
Lange, U. *et al, Z. Anorg. Allg. Chem.*, 1986, **542**, 207 (*synth*)

$Br_{24}H_6Sb_4$

IC-002260

Hexahydrogen tetracosabromotetraantimonate(*III,V*)

$H_6[Sb^{III}Br_6][Sb^{V}Br_6]_3$

M 2410.7

Hexapyridine salt: [19153-45-8].

Synth: $SbBr_3$ + Br_2 in HBr (aq.) + pyridine. Jet black (reflected light) to deep red (transmitted light) needle-like cryst. (HBr aq. containing trace H_2SO_4 and Br_2). Orthorhombic. Each cation is surrounded by two $[Sb^{III}Br_6]^{3\ominus}$ and four or six $[Sb^{V}Br_6]^{\ominus}$ anions.

Lawton, S.L. *et al, Inorg. Chem.*, 1971, **10**, 701 (*synth, cryst struct*)
Kidd, R.G. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 661 (*nmr*)
Donaldson, J.D. *et al, Inorg. Nucl. Chem. Lett.*, 1978, **14**, 93 (*mössbauer*)

IC-002261

$Br_{24}Ta_8$

Tantalum bromide (Ta_8Br_{24}), 8CI

[12514-63-5]

$[Ta_6Br_{12}][TaBr_6]_2$

M 3365.2
Thought to contain Ta_6Br_{12} octahedra. Synth. by melting $TaBr_4$ or by Al reduction of $TaBr_5$ in a 430-320° temp. gradient. Green solid.

Converse, J.G. *et al, Inorg. Chem.*, 1970, **9**, 1366 (*synth, ir*)

IC-002262

$Br_{42}Ta_{15}$

Tantalum bromide ($Ta_{15}Br_{42}$), 8CI

[12514-64-6]

$2Ta_6Br_{15}{\cdot}3TaBr_4$

M 6070.1
Synth. by heating $TaBr_4$ + $TaBr_5$ to 405-410° in a sealed tube. Brown solid. Paramagnetic μ_{eff} = 2.81 (295K), 2.31μ_B (77K).

Converse, J.G. *et al, Inorg. Chem.*, 1970, **9**, 1366 (*synth, ir, magnetism*)

IC-002263

C

Carbon

[7440-44-0]

C

M 12.0
Atomic No. 6; ground state electron config. $[He]2s^22p^2$. ^{12}C occurs in 98.9% natural abundance with ~1.1% ^{13}C, the latter being an important nmr nucleus. Elemental carbon occurs in cryst. and amorph. forms in the earth's crust. Manufactured forms include activated carbon, carbon black and coke. Carbon is widely distributed in the forms of fossil fuels (coal, gas, oil), as carbonaceous rocks (eg. limestone, dolomite), as atmospheric and dissolved CO_2. At least 6 crystalline forms known. Essential biological role: basis of all life. Abundance: 480 ppm earth's crust.

▷ FF5250100.

Diamond [7782-40-3]
Mineral. Diamond transforms into graphite above 1500° *in vacuo*. Giant molecule. Each C atom covalently bonded to 4 others tetrahedrally. For. C—C 154 pm. Hardest known substance. d 3.52. n_D 2.42. Hardness, Mohs' scale 10.

Graphite [7782-42-5]
Widely distributed in the earth's crust. Diamagnetic. Struct. comprises infinite layers of sp^2 C atoms in the form of hexagons lying in planes. Stacking arrangement ABAB. C—C 141.5 pm. Inter layer spacing 335.4 pm. Graphite also exists in an ABCABC stacking order (rhombohedral). Electrical cond. results from slight overlap of valency and conduction bands. Vast range of electrical and lubricating applications and as a moderator in thermal nuclear reactors. Highly refractory black solid, burns slowly in air above 450°. Forms many intercalation compds. with K, Rb, Cs and with many compds. Subl. 3850°. Triple pt. 3850°/120 atm. Other naturally occurring forms include Chaoite and Lonsdaleite.

Fullerene-C_{60} [99685-96-8]
Footballene. Buckminsterfullerene. Buckyball
C_{60} M 720.6
Truncated icosahedral (soccerball-shaped) struct., all 60 atoms equivalent in a rigid cage struct. formed of 5- and 6- membered rings. Ccp in solid state. Forms spontaneously when C is laser vapourised; in smoke from C arc. Forms metal-containing compds. which are superconductors, e.g. K_3C_{60}. Ultra stable mustard-coloured needles and plates. Sol. org-solvs. (magenta soln.). Mp >280°. ^{13}C nmr δ 143.2 (S) ppm.

Fullerene-C_{70} [115383-22-7]
[5,6]Fullerene-C_{70}
C_{70} M 840.7
Contains 5 different groups of C atoms in ratio 10:10:20:20:10. Elongated molecule with D_{5h} symmetry. Stacks in ccp or hcp from in solid state. Stable reddish brown solid or brown-black cryst. Sol. many org. solvs. esp. aromatic solvs. (port-wine coloured). Mp >280°. Closely related is a cylindral form nick-named Buckytubes. ^{13}C nmr-5 peaks.

[1333-86-4, 12070-15-4, 12075-35-3, 12184-80-4, 12595-82-3, 12595-84-5, 14333-33-6, 14762-74-4, 14762-75-5, 15578-67-3, 15578-68-4, 15776-26-8, 15929-23-4, 16449-60-8, 21360-00-9, 26062-64-6, 26160-40-7, 30852-91-6, 35284-81-2, 35284-82-3, 35284-83-4, 40436-13-3, 52015-77-7, 52015-78-8, 52015-79-9, 67771-13-5, 81793-67-1, 101126-49-2, 112303-18-1, 115383-19-2, 115383-20-5, 115383-21-6, 118619-69-5, 118678-75-4]

Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1924, **5**, 710 (*bibl*)
Inorg. Synth., 1946, **2**, 74 (*synth, sugar charcoal*)
Weeks, M.E., *Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 3, 75 (*history*)
Hennig, G.R., *Prog. Inorg. Chem.*, 1959, **1**, 125 (*graphite compds, rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1967, **B1-B3**; 1970, **C1-C4**; 1971, **D1-D6** (*isotopes, bibl*)
Mantell, C.L., *Carbon and Graphite Handbook*, Interscience, 1968.
Bruton, E., *Diamonds*, NAG Press, 1970.
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 1173 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 609.
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 556 (*rev, phase diagram*)
Selic, H. *et al, Adv. Inorg. Chem. Radiochem.*, 1981, **23**, 281 (*rev, intercalation compds*)
Stankevich, I.V. *et al, Russ. Chem. Rev.* (*Engl. Transl.*), 1984, **53**, 640 (*cryst C*)
Curl, R.F. *et al, Science* (*Washington, D.C.*), 1988, **242**, 1017 (*rev, fullerenes*)
Taylor, R. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 1423 (C_{60}, *synth, ms, cmr, ir, uv*)
Ajie, H. *et al, J. Phys. Chem.*, 1990, **94**, 8630 (C_{70}, *synth, ir, cmr, uv-vis*)
Kraetschmer, W. *et al, Nature* (*London*), 1990, **347**, 354 (C_{60}, C_{70}, *synth, props*)
Kroto, H. *et al, Pure Appl. Chem.*, 1990, **62**, 407 (*rev, fullerenes*)
Baum, R.M., *Chem. Eng. News*, 1991, 31 (*rev, fullerenes*)
Iijima, S. *et al, Nature* (*London*), (7 November), 1991, 56 (*cylindrical form*)
Hebard, A.F. *et al, Nature* (*London*), 1991, **350**, 600 (K_3C_{60})
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 110 (*haz*)

CAgN

Silver(*I*) cyanide (AgCN)

IC-002264

Argentous cyanide

[506-64-9]

AgCN

M 133.8
Struct. comprises infinite linear chains of metal atoms linked through CN groups. Prepd. by adding aq. KCN or NaCN to aq. $AgNO_3$. Used in silver plating; formerly used for prep. of dil. HCN by treatment with HCl. White or greyish, odourless powder. Stable in dry air. Darkens on exp. to light. Insol. H_2O, alcohols, dil. acids. Sol. aq. alkali cyanides, boiling conc. HNO_3. Dec. at 320°.

▷ Deadly poison. Skin and severe eye irritant. VW3850000.

Baker, H.B. *et al, J. Chem. Soc.*, 1926, 2527 (*cryst struct*)
Cook, J.R.P. *et al, J. Chem. Soc.*, 1935, 1001 (*synth*)
Težak, B., *Z. Phys. A*, 1935, **A175**, 219 (*synth*)
German, W.L., *J. Chem. Soc.*, 1938, 1027 (*synth*)
Stalicup, W.D. *et al, J. Chem. Phys.*, 1942, **10**, 199 (*ir*)
Gallais, F., *Bull. Soc. Chim. Fr.*, 1945, **12**, 657 (*uv*)
El Sayed, M.F.A. *et al, J. Inorg. Nucl. Chem.*, 1958, **6**, 187 (*ir*)
Pistorius, G.W.F.T., *J. Inorg. Nucl. Chem.*, 1961, **19**, 367 (*cryst struct*)
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, **1**, 661 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1006 (*use*)
Kalani, D.K., *Lab. Pract.*, 1968, **17**, 691 (*magnetism*)
Merck Index, 11th Ed., 1989, No. 8458.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3029.

CAgNS

Silver(*I*) thiocyanate

IC-002265

[1701-93-5]

AgSCN

M 165.9
Precipitated from aq. solns. of $Ag^{\oplus}$ + $NCS^{\ominus}$. Commercially available. Colourless cryst. Struct. is polymeric consisting of zigzag —Ag—N≡C—S— chains.

Lindqvist, I., *Acta Crystallogr.*, 1957, **10**, 29 (*cryst struct*)
Kinell, P.O. *et al, Acta Chem. Scand.*, 1959, **13**, 1607 (*ir, raman*)
Inorg. Synth., 1966, **8**, 27 (*synth*)
Smith, D.L. *et al, J. Appl. Crystallogr.*, 1982, **15**, 488 (*cryst struct*)

CAg_2O_3

Silver(*I*) carbonate (Ag_2CO_3)

IC-002266

[534-16-7]

Ag_2CO_3

M 275.7
There is evidence of large anisotropic vibration of the Ag atoms. Light yellow monoclinic powder. Darkens on drying and exp. to light. Spar. sol. H_2O. Readily sol. dil. aq. nitric acid, ammonia, alkali cyanides. Dec. at about 220° into Ag_2O and CO_2, and at higher temps. into metallic silver. ΔH_f° −508.1 kJ mol^{-1}, ΔG_f° −439.6 kJ mol^{-1}.

Donohue, J. *et al, J. Am. Chem. Soc.*, 1944, **66**, 2472 (*theory*)
Inorg. Synth., 1957, **5**, 19 (*synth*)
U.S. Pat., 3038803, (1962) (*use*)
Rous, S.D. *et al, Spectrochim. Acta*, 1964, **20**, 781 (*ir*)
Masse, R., *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 1428 (*cryst struct*)
Merck Index, 11th Ed., 1989, No. 8453.

[CAlN]

Aluminium carbide nitrides

IC-002267

Aluminium carbonitride

Aluminium carbide nitride (Al_4C_3N) [12180-19-7]
C_3Al_4N M 184.9
Struct. is related to AlN and Al_4C_4 with tetrahedral coordn. of N, tbp or octahedral carbon, and 4-coord. Al. Synth. from AlN in C crucible in N_2 at 2000°.

Aluminium carbide nitride ($Al_6C_3N_2$)
$C_3Al_6N_2$ M 225.9
Other related compds. include $Al_7C_3N_3$ and $Al_8C_3N_4$.

Stackelberg, M.V. *et al, Z. Physik. Chem.*, 1935, **175**, 127 (*synth*)
Jeffrey, G.A. *et al, Acta Crystallogr.*, 1963, **16**, 559; 1966, **20**, 538 (*synth, cryst struct*)

[CAlO]

Aluminium carbide oxide

IC-002268

Aluminium oxycarbide

Aluminium carbide oxide (Al_4CO_4) [12011-53-9]
CAl_4O_4 M 183.9
$Al(O_3C)$ tetrahedra share edges and corners. Synth. from Al_2O_3 + Al_4C_3 at 1800°. Colourless transparent laths.

Aluminium carbide oxide (Al_2CO) [12011-50-6]
CAl_2O M 81.9
May be formulated as $[AlO]_n[Al_2C_2]_n[AlO]_n$ with long-range disorder. Struct. related to wurtzite. Synth. from Al_2O_3 + Al_4C_3 at 2000°. Hexagonal needles.

Foster, L.M. *et al, J. Am. Chem. Soc.*, 1956, **39**, 1 (*synth, powder struct, Al_2OC*)
Long, G. *et al, J. Am. Ceram. Soc.*, 1961, **44**, 255 (*phase diagram*)
Amma, E.L. *et al, J. Chem. Phys.*, 1961, **34**, 252 (*cryst struct, Al_2OC*)
Jeffrey, G.A. *et al, Acta Crystallogr.*, 1963, **16**, 177; 1966, **20**, 538 (*cryst structs*)
Cox, J.H. *et al, Can. J. Chem.*, 1963, **41**, 1414 (*powder struct*)

$CAl_6CaNa_6O_{27}Si_6$

Cancrinite

IC-002269

[12172-98-4]

$Na_6Ca[Al_6Si_6O_{24}][CO_3]{\cdot}2H_2O$

M 952.4
Zeolite struct. CAN with 1-D channels (590 pm across) and $(AlSi—O)_{12}$ rings. Mineral. Synth. from Na_2CO_3—Al_2O_3—SiO_2 aq. gel at 80-400°. Absorbs Ne, Ar, Kr. White hexagonal prisms (aq. melt). Aluminogermanate and gallosilicate analogues also descr. $CO_3^{2\ominus}$ may be replaced e.g. by $SO_4^{2\ominus}$ $NO_3^{\ominus}$.

Barrer, R.M. *et al, J. Chem. Soc.*, 1952, 1561; 1964, 485; *J. Chem. Soc. A*, 1970, 1523 (*synth*)
Barrer, R.M. *et al, Proc. R. Soc. London*, 1956, **236**, 227 (*ion exch*)
Litvin, B.N. *et al, Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1962, **6**, 643 (*synth*)
Jarchow, O., *Z. Kristallogr.*, 1965, **122**, 407 (*cryst struct*)
Barrer, R.M. *et al, J. Phys. Chem. Solids*, 1971, **32**, 731 (*absorption*)
Klinowski, J. *et al, J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Pabst, N.B. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 893 (*cryst struct*)
Fyfe, C.A. *et al, J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)

Belokoneva, E.L. *et al, Soc. Phys. Crystallogr. (Engl. Transl.)*, 1986, **31**, 516 (*cryst struct*)
Meier, W.M. *et al, Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 40.

IC-002270

CAsV$_3$
Vanadium arsenide carbide (V$_3$AsC), 8CI
[12127-23-0]

V_3AsC

M 188.8
Cr_3AlC-like struct. Synth. by heating the elements to 1100°.

Boller, H. *et al, Monatsh. Chem.*, 1966, **97**, 1053.

IC-002271

CAsV$_3$
Vanadium arsenide carbide (V$_3$AsC), 8CI

V_3AsC

M 239.7
C is in octahedral sites of the V_3As lattice (latter related to Re_3B). Synth. by heating the elements to 1100°.

Boller, H. *et al, Monatsh. Chem.*, 1967, **98**, 2127 (*synth, cryst struct*)

IC-002272

CAuClO
Carbonylchlorogold, 9CI
Gold carbonyl chloride
[50960-82-2]

Au(CO)Cl

M 260.4
Useful starting material for synthesising Au(I) compounds. Moisture-sensitive sublimable cryst. Stable to 110°. Sol. C_6H_6, toluene, CH_2Cl_2, CCl_4, $SOCl_2$, THF. Subl. 95°. Extremely reactive to water. CO lost when treated with Py, PPh_3, CNC_6H_{11} etc. Ir ν_{CO} 2153 cm^{-1} (C_6H_6).

Manchot, W. *et al, Ber.*, 1925, **58**, 2175 (*synth*)
Kharasch, M.S. *et al, J. Am. Chem. Soc.*, 1930, **52**, 2919 (*synth*)
Belli Dell'Amico, D. *et al, Gazz. Chim. Ital.*, 1973, **103**, 1099.
Jones, P.G. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1434 (*mossbauer*)
Browning, J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*nmr, ir*)
Inorg. Synth., 1986, **24**, 236 (*synth*)

IC-002273

CAuN
Gold(*I*) cyanide (AuCN), 9CI
Cyanogold. Aureux cyanide
[506-65-0]

AuCN

M 222.9
Commercially available. Lemon-yellow cryst. powder. Stable in air. Unstable to light when moist. Spar. sol. H_2O, sol. alkali cyanide solns.

▷ Highly toxic.

Isocyanomethane complex: [60974-77-8]. *(Cyano-C)(isocyanomethane)gold. Cyano(methyl isocyanide)gold*(1)
$C_2H_3AuN_2$ M 264.0
Colourless plates. Insol. H_2O, common org. solvs. In solid state linear molecules pack parallel to each other. Interatomic distances: Au—Au 352-372 pm.
PEt_3 complex: see *Cyano(triethylphosphine)gold, IC-005772*
PPh_3 complex: see *Cyano(triphenylphosphine)gold*(1), *IC-010256*

Arai, G., *Bull. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1962, **81**, 307 (*synth, deriv*)
Chadwick, B.M. *et al, Adv. Inorg. Chem. Radiochem.*, 1968, **8**, 156 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-81, **2**, 1018.
Esperas, S., *Acta Chem. Scand., Ser. A*, 1976, **30**, 527 (*deriv, cryst struct*)

[CB]

IC-002274

Boron carbides
Carbon borides
Several phases reported eg. $B_{50}C$, $B_{26}C_2$, $B_{25}C_2$, $B_{22}C_3$, B_4C in addition to B_4C ($B_{12}C_3$) and also BC, BC_2, and B_2C.

Boron carbide (B_4C), 9CI, 8CI [12069-32-8]
Carbon tetraboride
C_4B M 58.8
Rhombohedral cell. Struct. similar to that of rhombohedral B. Each B atom is bonded to 5 others in an icosahedron, as well as to either a C or B atom in an adjacent icosahedron. Synth. from B_2O_3 in a graphite furnace at 1400-1850°; $BCl_3 + CCl_4$ under H_2 at 1200-2000°; $BCl_3 + CH_4$ at 1900°; $B_2O_3 + Mg + C$ at 1000-1200°. An abrasive (hardness approaching that of diamond); fuel element in nuclear reactors; material for lightweight armour; used to manuf. refractory briquettes. Available as a fibre. Dark grey, almost black, needles and plates, with metallic lustre. Mp 2450° (2350°). Low density, high strength material with good thermal and chemical stability. Resistant to most acids. Rapidly attacked by molten alkali. Semiconductor. Attacked by $HNO_3 + H_2SO_4 + HF$. Hydrolysed (H_2O) at 800-950° → $B_2O_3 + C + H_2$. Oxidised in air at 800-1000°.

[12075-36-8]

Verhaegen, G. *et al, J. Chem. Phys.*, 1964, **40**, 1622 (*ms*)
Economy, J., *Chem. Eng. Progress*, 1965, **65**, 46 (*rev, uses*)
Prickett, R.L. *et al, Adv. X-Ray Anal.*, 1967, **10**, 221 (*struct*)
Mierzejewska-Appenheimer, S. *et al, J. Phys. Chem. Solids*, 1967, 229 (*synth*)
Borchert, W. *et al, Krist. Tech.*, 1969, **4**, 293 (*single cryst*)
Ashbee, K.H.G., *Acta Metall.*, 1971, **19**, 1079 (*struct*)
Kieffer, R. *et al, Ber. Dtsch. Keram. Ges.*, 1971, **48**, 385 (*synth, phase diagram*)
Hynes, T.V. *et al, J. Chem. Phys.*, 1971, **54**, 5296 (*B-11 nmr*)
Motoc, C. *et al, J. Crystal Growth*, 1973, **18**, 29 (*synth*)
Becher, H.J. *et al, Z. Anorg. Allg. Chem.*, 1974, **410**, 274 (*ir*)
Thompson, R., *J. Less-Common Met.*, 1976, **47**, 279 (*rev*)
Rovner, J.H. *et al, Nucl. Technol.*, 1976, **29**, 274 (*rev*)
Boron and Refractory Borides, (Ed. Matkovich, V.I.), Springer-Verlag, Berlin, 1977 (*rev, bibl*)
Thevenot, F. *et al, Ind. Ceram.*, 1979, 655, 739 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *Suppl. Vol.*, 1981, 2, 117 (*rev, bibl*)
Bouchacourt, M. *et al, J. Less-Common Met.*, 1981, **82**, 227 (*synth, ir, props, cryst struct*)
Reinmuth, K. *et al, J. Nucl. Mater.*, 1984, **124**, 175 (*rev, props, uses*)

IC-002275

CBCl$_2$NO
Dichloro(isocyanato)borane, 9CI
Dichloroboron isocyanate
[55969-82-9]

$Cl_2B—NCO$

M 123.7

Unstable colourless gas.

Mongeot, H. *et al, J. Mol. Struct.*, 1980, **62**, 35 (*synth, ir*)
Alsse, M. *et al, J. Chem. Soc., Dalton Trans.*, 1990, 1569 (*pe*)

CBF$_2$O **IC-002276**
Carbonyltrifluoroboron, 10CI
Trifluoroborane carbonyl. Trifluoroborane, compd. with carbon monoxide (1/1), 9CI. Boron trifluoride carbonyl
[51006-66-7]

$F_2B—CO$

M 95.8
Weakly bound complex studied by matrix isol. methods.

Horvick, S.F. *et al, J. Am. Chem. Soc.*, 1973, **95**, 8547
Archibald, R.M. *et al, J. Chem. Soc., Faraday Trans. 2*, 1973, **69**, 1793 (*struct*)
Janda, K.C. *et al, J. Am. Chem. Soc.*, 1978, **100**, 8074 (*struct*)
Armstrong, D.R., *Inorg. Chim. Acta*, 1979, **34**, 177 (*struct*)
Clark, D.T. *et al, Chem. Phys.*, 1980, **46**, 43.

CBF$_4^-$ **IC-002277**
Trifluoro(trifluoromethyl)borate(1−), 10CI, 9CI
(Trifluoromethyl)trifluoroborate

$[F_3CBF]^-$

M 136.8 (ion)
K salt: [42298-15-7].
Monoclinic cryst. (EtOH).

Jaskovitz, J.F. *et al, Appl. Spectrosc.*, 1973, **27**, 209 (*ir, raman*)
Brauer, D.J. *et al, Inorg. Chem.*, 1977, **16**, 2305 (*ir, raman, synth, cryst struct*)
Pawelke, G. *et al, J. Organomet. Chem.*, 1979, **178**, 1 (*synth*)

CBMo$_2$ **IC-002278**
Molybdenum boride carbide (Mo_2BC)
[12179-61-2]

Mo_2BC

M 214.7
Orthorhombic cell, carbon is octahedrally coord. by Mo and B has trigonal prismatic coord. and forms chains as in CrB. Obt. by arc-melting appropriate amounts of Mo metal filings, boron and carbon (as graphite) in a gettered Ar atm. V. hard solid. Insol. Mp ~2800°.

Jeitschko, W. *et al, Monatsh. Chem.*, 1963, **94**, 65 (*struct*)
Smith, S.G. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 698 (*struct, synth*)

CBNb$_2$ **IC-002279**
Niobium boride carbide (Nb_2BC), 11CI
[81030-29-7]

Nb_2BC

M 208.6
Phases $Mo_{2-x}Nb_xBC$ are known for $0 \leqslant x \leqslant 0.80$. Isostructural with Mo_2BC. Only known as a solid soln. in Mo_2BC. Synth. by arc-melting Mo + Nb + B + C.

Lejay, P. *et al, J. Less-Common Met.*, 1981, **82**, 193 (*synth, struct, magnetism*)

CBTa$_2$ **IC-002280**
Tantalum boride carbide (Ta_2BC), 11CI
[81030-31-1]

Ta_2BC

M 384.7
Synth. by dissolving B in Ta. Solid solns. $Mo_{1-x}Ta_xBC$ ($0 < x < 0.35$) may be synth. by arc-melting the components. Possesses same unit cell parameters as Ta, but is much harder.

[67954-27-2]

Rudy-Kieser, H.J. *et al, C.A.*, 1978, **89**, 147946w (*synth*)
Lejay, P. *et al, J. Less-Common Met.*, 1981, **82**, 193 (*synth, solid solns*)

CBZr$_2$ **IC-002281**
Zirconium boride carbide (Zr_2BC), 11CI
Dizirconium boride carbide
[81030-33-3]

Zr_2BC

M 205.2
This phase is only known as solid solns. in Mo_2BC. The composition range in $Mo_{2-x}Zr_xBC$ is $0 \leqslant x \leqslant 0.35$. Struct. comprises layers of edge-sharing MC_6 octahedra; these layers are separated by layers of boron atoms which form zig-zag chains through trigonal prisms of M atoms. Synth. by arc-melting Mo + Zr + B + C in an argon atm. The various phases are superconducting with T_c between 6 and 7K.

Lejay, P. *et al, J. Less-Common Met.*, 1981, **82**, 193 (*synth, superconductivity*)

CB$_2$F$_4$O **IC-002282**
Hexafluorotetraborane carbonyl
Boron fluoride (B_2F_4) compd. with carbon monoxide (1/1)
[12244-49-4]

$(F_2B)_2B—CO$

M 185.2
Solid. Sol. CCl_3F. Mp 40°.

Timms, P.L., *J. Am. Chem. Soc.*, 1967, **89**, 1629 (*synth, ir, ms, F-19 nmr*)
Kirk, R.W. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1392 (*synth*)

CBaNa$_2$Nd$_2$O$_{16}$Si$_4$ **IC-002283**
Barium neodymium sodium carbonate silicate ($BaNd_2Na_2(CO_3)(Si_2O_{13})$)

$Na_2BaNd_2[Si_2O_{13}][CO_3]$

M 836.1
Synthetic monocyclosilicate (4 SiO_4 tetrahedra per ring). Na, Nd octahedral, Si tetrahedral, Ba hendecahedral, C trigonal planar. Cryst.

Malinovskii, Yu.A., *Sov. Phys.-Dokl. (Engl. Transl.)*, 1983, **28**, 829 (*cryst struct*)

CBaO$_3$ **IC-002284**
Barium carbonate ($BaCO_3$)
Carbonic acid, barium salt, 8CI
[513-77-9]

$BaCO_3$

M 197.3
Struct. resembles aragonite ($CaCO_3$). Synth. by addition of aq. $[NH_4]HCO_3$ to aq. $BaCl_2$ at ⩽ 45°. Commercially available. Rat poison. Used in prep. of $YBa_2Cu_3O_{7-x}$ high transition temp. superconductors. White orthorhombic cryst.; becomes hexagonal at 803° and cubic at 976°. Dec. on heating by CO_2 loss. Dissolves in

acids to form corresp. Ba salts. Prac. insol. H_2O (2.2×10^{-3} g per 100 cm^3 at 18°; 6.5×10^{-2} g per 100 cm^3 at 100°); insol. EtOH. Mp 1740° (90 atm.). ΔH_f° −1216 kJ mol^{-1}; ΔG_f° −1138 kJ mol^{-1}; S° 112 J K^{-1} mol^{-1}.

▷ Highly toxic. Irritant. CQ8600000.

Mineral-form [14941-39-0]

Witherite

Found as low-temp. mineral in hydrothermal vein deposits. Pseudo-hexagonal dipyramids, white, sometimes with pale yellow, greenish or brown tinge

Lander, J.J., *J. Chem. Phys.*, 1949, **17**, 892 (*cryst struct.* polymorphs)
Khrishnamurti, D., *Proc. - Indian Acad. Sci., Sect. A*, 1960, **51**, 285 (*raman*)
Ross, S.D. *et al, Spectrochim. Acta*, 1964, **20**, 781 (*ir*)
Muyskens, D.J. *et al, Encycl. Chem. Process. Des.*, 1977, **4**, 50 (*bibl*)
Japan. Pat., 80 20 229, (1980); *CA*, **93**, 49674 (*synth*)
Fahim, R.B. *et al, Powder Technol.*, 1982, **33**, 161 (*thermal dec*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 333B (*haz*)

CBi_2O_5 IC-002285

μ-[Carbonato(2−)-*O*:*O*']bis[dioxodibismuth], 9CI

(Carbonato)dioxodibismuth, 8CI. (μ-Carbonato) dioxodibismuth, 8CI. Bismuth carbonate oxide. [Carbonylbis(oxy)]bis[oxobismuthine], 10CI

$(BiO)_2CO_3$ (approx. composition)

M 509.9

Contains variable amounts of water. Synth. $Bi(NO_3)_3$ + Na_2CO_3 in soln. Veterinary and other medical uses (mild astringent). Also used in ceramics to give pearly surfaces. Odourless, tasteless, white powder. Practically insol. H_2O. Sol. mineral acids. On heating, gives Bi_2O_3.

Mineral-form [12069-37-3]

Bismutite

Tetragonal layer struct. A commonly occuring secondary mineral. Found in Europe, USSR, S. Africa, S. America, Australia (N.S. Wales) and is particularly widespread in the USA. Straw-coloured to brownish-yellow vitreous cryst. Contains small amounts H_2O.

Gmelin Handbook Inorg. Chem., Syst. No. 19, 1927, 178; 1964, 829.
Hunt, J.M. *et al, Anal. Chem.*, 1950, **22**, 1478 (*ir*)
Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1951, **II**, 259.
Wesolowski, M., *Arzneim.-Forsch.*, 1978, **28**, 372 (*rev, synth, anal, uses*)
Fontaine-Bienfait, J. *et al, Sci. Tech. Pharm.*, 1978, **7**, 9 (*pharmacol, rev*)

$CBrClF_2$ IC-002286

Bromochlorodifluoromethane, 9CI

Fluorocarbon 12B1. Halon 1211. BCF

[353-59-3]

F_2CClBr

M 165.3

Manuf. by bromination of $CHClF_2$. Used as refrigerant and in fire extinguishing. Gas. d_{15} 1.850. Fp −160.5°. Bp −4°.

▷ Dec. to toxic carbonyl halides on strong heating in the presence of air. Production controlled by environmental legislation. PA5270000.

Haszeldine, R.N., *J. Chem. Soc.*, 1952, 4259 (*synth*)
Glew, D.N., *Can. J. Chem.*, 1960, **38**, 208 (*props*)
El-Sabban, M.Z. *et al, J. Mol. Spectrosc.*, 1967, **22**, 23 (*props*)
Grunwald, E. *et al, J. Org. Chem.*, 1979, **44**, 2377 (*synth*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 561.

CBrClO IC-002287

Carbonyl bromide chloride, 8CI

Carbonic bromide chloride, 11CI, 9CI. Carbonyl chlorobromide

[7726-12-7]

O=CBrCl

M 143.3

Faintly yellow, hygroscopic liq. d^{15} 1.82. Bp 25°.

▷ Highly toxic.

Oxime.

CHBrClNO M 158.3

Mp 36°.

v. Bartal, A., *Justus Liebigs Ann. Chem.*, 1906, **345**, 334 (*synth*)
Patty, R.R. *et al, Spectrochim. Acta*, 1959, 60 (*ir*)
Evans, J.C. *et al, Trans. Faraday Soc.*, 1959, **55**, 1817 (*synth, spectra*)
Biryukov, I.P. *et al, CA*, 1968, **68**, 44645 (*nqr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 224 (*synth*)
Gombler, W., *Spectrochim. Acta, Part A*, 1981, **37**, 57 (*cmr*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 490.

CBrClS IC-002288

Thiocarbonyl bromide chloride

Carbonothioic bromide chloride, 9CI

[35907-57-4]

S=CBrCl

M 159.4

Obt. contaminated with CS_2 and COS.

Middleton, W.J. *et al, J. Org. Chem.*, 1965, **30**, 1375.
Brema, J.L. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 809 (*ir, raman, synth*)
Sombler, W., *Spectrochim. Acta, Part A*, 1981, **37**, 57 (*nmr*)

$CBrCl_2F$ IC-002289

Bromodichlorofluoromethane, 9CI, 8CI

Fluorocarbon 11B1. Halon 1121

[353-58-2]

$CBrCl_2F$

M 181.8

Fire extinguishing agent, solvent. Liq. d_{22} 1.95. Bp 52.8°.

Haszeldine, R.N., *J. Chem. Soc.*, 1952, 4265 (*synth*)
U.S. Pat., 2 716 668, (1955); *CA*, **50**, 7845e.
U.S. Pat., 2 755 314, (1956); *CA*, **51**, 2016 (*manuf*)
Gilbert, R.L. *et al, J. Chem. Phys.*, 1960, **33**, 1872 (*ir, raman*)

$CBrCl_3$ IC-002290

Bromotrichloromethane, 9CI

Trichloromethyl bromide

[75-62-7]

$CBrCl_3$

M 198.2

Solv. for Hunsdiecker reacns., reagent for photobrominations and carbene generation. Liq. d_4^{20} 2.01. Fp −5.8°. Bp 104.2°.

▷ Hepatotoxin. PA5400000.

Wouters, J., *CA*, 1935, **29**, 2849 (*synth*)
Zakharkin, L.I., *CA*, 1954, **48**, 547 (*synth*)
Delwaulle, M.L. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1195 (*raman*)
Lehmann, G. *et al, J. Prakt. Chem.*, 1963, **22**, 230 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 80; **7**, 40.
Tsyashchenko, Y.P. *et al, CA*, 1972, **77**, 11913 (*struct*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 580.

CBrFO IC-002291

Carbonic bromide fluoride, 9CI

Carbonyl bromide fluoride. Bromofluorophosgene

[753-56-0]

O=CBrF

M 126.9

Formed from $CFBr_3$ + SO_3. Gas, thermally stable to 125°. Rapidly hydrol. to CO_2 + HBr + HF. Mp −120°. Bp −17° to −10°.

Patty, R.R. *et al, Spectrochim. Acta*, 1959, **15**, 60 (*ir*)
Siegemund, G., *Angew. Chem., Int. Ed. Engl.*, 1973, **12**, 918 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 224 (*synth*)

$CBrF_2N$ IC-002292

Bromocarbonimidic difluoride

N-Bromo-1,1-difluoromethanimine, 9CI. N-Bromodifluoroformimide

[90624-74-1]

$F_2C{=}NBr$

M 143.9

Formed from $FC{\equiv}N$ + KF + Br_2 at 22°. Pale yellow gas. Mp −93° to −92°. Bp 14.5°.

O'Brien, B.A. *et al, J. Am. Chem. Soc.*, 1984, **106**, 4266 (*synth, ir, raman, F-19 nmr, uv*)
Bauknight, C.W. *et al, J. Org. Chem.*, 1988, **53**, 4443 (*synth*)

$CBrF_3$ IC-002293

Bromotrifluoromethane, 9CI, 8CI

Fluorocarbon 13B1. Halon 1301

[75-63-8]

$CBrF_3$

M 148.9

Synth. by bromination of CHF_3. Fire extinguishing agent, refrigerant, chemical intermed. Gas. d_{21} 1.58. Fp −168°. Bp −57.8°, Bp −59°.

▷ Toxic, irritant. Production regulated by environmental legislation. PA5425000.

Haszeldine, R.N., *J. Chem. Soc.*, 1951, 584 (*synth*)
Hauptschein, M. *et al, J. Am. Chem. Soc.*, 1952, **74**, 1347 (*synth*)
Stuckey, W.K. *et al, Nature (London)*, 1966, **211**, 963 (*ms*)
Gallant, R.W., *Hydrocarbon Process.*, 1968, **47**, 128 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 42.
de Marco, R.A. *et al, J. Magn. Reson.*, 1975, **18**, 522 (*cmr*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 277.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 581.

$CBrF_3S$ IC-002294

Trifluoromethanesulfenyl bromide, 9CI

[753-92-4]

F_3CSBr

M 180.9

Orange-red liq. d_4^{15} 1.770. Bp 36°. n_D^{15} 1.3855. Dec. by sunlight to Br_2 and CF_3SSCF_3.

Yarovenko, N.N. *et al, Zh. Obshch. Khim.*, (*Engl. transl.* p. 3749), 1959, **29**, 3786 (*synth*)
Ratcliffe, C.T. *et al, J. Am. Chem. Soc.*, 1968, **90**, 5403 (*synth, F nmr, ir*)
Altabef, A.B. *et al, Z. Anorg. Allg. Chem.*, 1983, **506**, 161 (*synth, ir, raman, props*)
Minkwitz, R. *et al, Z. Anorg. Allg. Chem.*, 1985, **527**, 161; **531**, 31 (*synth, ir, raman, F nmr, cmr, uv*)

$CBrF_3Se$ IC-002295

Trifluoromethaneselenenyl bromide

Selenohypobromous acid trifluoromethyl ester. Trifluoromethyl selenohypobromite

[753-95-7]

F_3CSeBr

M 227.8

Formed from $(CF_3Se)_2$ + Br_2. Colourless liq. Hydrol. to $(CF_3)_2Se_2$. Bp 57°.

Dale, J.W. *et al, J. Chem. Soc.*, 1958, 2939 (*synth*)
Marsden, C.J., *J. Fluorine Chem.*, 1975, **5**, 401 (*synth, ir, raman, F-19 nmr*)
Clase, H.J. *et al, Can. J. Spectrosc.*, 1977, **22**, 92 (*ir*)
Gombler, W., *Z. Naturforsch., B*, 1981, **36**, 535 (*nmr*)
Gombler, W., *J. Am. Chem. Soc.*, 1982, **104**, 6616 (*Se-77 nmr*)

CBrHgN IC-002296

Mercury bromide cyanide (HgBr(CN))

[52904-61-7]

HgBr(CN)

M 306.5

Obt. in soln. in equilibrium with $HgBr_2$ and $Hg(CN)_2$ at 20°. Sol. THF, DMSO, Py; insol. H_2O.

Belevantsev, V.I. *et al, Koord. Khim.*, 1980, **6**, 1000 (*uv-vis*)
Peringer, P. *et al, Inorg. Nucl. Chem. Lett.*, 1980, **16**, 205 (*Hg-199 nmr*)
Beck, M.T. *et al, React. Kinet. Catal. Lett.*, 1974, **1**, 125 (*formn*)
Goggin, P.L. *et al, J. Chem. Res. (S)*, 1979, 194 (*cmr, Hg-199 nmr*)
Delwaulle, M.-L., *Bull. Soc. Chim. Fr.*, 1940, **7**, 359 (*raman*)

CBrN IC-002297

Cyanogen bromide

Bromine cyanide

[506-68-3]

$BrC{\equiv}N$ ($C_{\infty v}$)

M 105.9

Interatomic distances: Br—C 179, C—N 115.7 pm. Commercially available. Used in the Von Braun reaction, cleavage of thioethers, synth. of heterocycles, synth. of *trans* olefins, synth. of disulfides, phenol dehydroxylation, synth. of 1,2-aminocarbonates, synth. of cyanatobenzene. Cryst. Sol. Et_2O, H_2O, EtOH. d_4^{20} 2.01. Mp 52°. Bp 61-62°.

▷ Highly toxic, irritant. GT2100000.

Fieser and Fieser, Reagents for Organic Synthesis, **1**, 174; **2**, 93; **4**, 110; **5**, 169; **6**, 148; **8**, 131; **9**, 127 (*uses*)

Cook, R.P., *J. Chem. Soc.*, 1935, 1001 (*synth, props*)
Org. Synth., Coll. Vol., 2, 1943, 150 (*synth*)
Tyler, J.K. *et al, Trans. Faraday Soc.*, 1963, **59**, 2661 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 632 (*synth*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 987.

CBrNO — IC-002298

Bromine isocyanate

[3644-72-2]

$BrN{=}C{=}O$

M 121.9
Synth. from Br_2 + AgCNO at 150°. V. moisture-sensitive yellow cryst., at low temp. melting to brown liq. which rapidly dimerises to $Br_2NC(O)NCO$ at −40°. Mp −48°.

▷ Explosive.

[91914-88-4, 91914-89-5]

Gottardi, W., *Angew. Chem., Int. Ed. Engl.*, 1971, **10**, 416 (*synth, ir*)
Jemson, H.M. *et al, Chem. Phys. Lett.*, 1984, **108**, 496 (*microwave*)

CBrNS — IC-002299

Bromine thiocyanate

Thiocyanogen bromide

[29284-59-1]

$N{\equiv}CSBr$

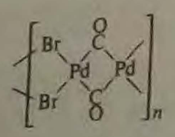
M 137.9
Interatomic distances: Br—S 218.0, N—C 115.6, S—C 170.1 pm; angle: BrSC 99.8°. Formed from $Pb(SCN)_2$ + Br_2 or $(SCN)_2$ + Br_2. Colourless cryst. Sublimable but readily dec. to Br_2.

Nelson, M.J. *et al, J. Chem. Soc.*, 1960, 604 (*synth, ir*)
Frost, D.C. *et al, J. Am. Chem. Soc.*, 1981, **103**, 4423 (*synth, pe*)
Jemson, H.M. *et al, Can. J. Chem.*, 1987, **65**, 2478 (*synth, microwave*)

CBrOPd — IC-002300

Bromocarbonylpalladium, 10Cl, 9Cl

[43732-38-3]



M 214.3
Polymeric. Catalyses carbonylation of phenols. Yellow solid or green solid. Darkens at 145°, to black at 200°.

[31691-41-5]

Colton, R. *et al, Aust. J. Chem.*, 1973, **26**, 2607 (*synth, ir*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 534 (*synth, ir*)

CBrORu — IC-002301

Bromo(carbonyl)ruthenium(*I*)

$[Ru(CO)Br]_n$

M 208.9
Polymeric as solid; struct. unknown. Prepd. by treating $RuBr_3$ with CO (350 atm.; 180°). Colourless cryst. Insol. org. solvs. Dec. at 200° to give Dibromodicarbonylruthenium, IC-002839 and Ru metal. Dec. in H_2O and acid; reduces Ag(*I*).

Manchot, W. *et al, Chem. Ber.*, 1930, **63**, 1635 (*synth*)

CBr_2ClF — IC-002302

Dibromochlorofluoromethane, 9Cl, 8Cl

Fluorocarbon 11B2. Halon 1112

[353-55-9]

Br_2CClF

M 226.2
Fire extinguishing agent, solvent. Liq. d^{22} 2.32. Bp 79.5-80.5°.

Haszeldine, R.N., *J. Chem. Soc.*, 1952, 4265 (*synth*)
U.S. Pat., 2 716 668, (1955); *CA*, **51**, 2016i (*manuf*)

CBr_2Cl_2 — IC-002303

Dibromodichloromethane, 9Cl

R 10B2

[594-18-3]

CCl_2Br_2

M 242.7
d_0^{25} 2.42. Mp 38° (22°). Bp 150.2° (135°). Turns yellow on exp. to light.

Arnold, M., *Justus Liebigs Ann. Chem.*, 1887, **240**, 208 (*synth*)
Volkringer, H. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1937, **204**, 1927 (*synth*)

CBr_2F_2 — IC-002304

Dibromodifluoromethane

Fluorocarbon 12B2. Halon 1202. Difluorodibromomethane

[75-61-6]

CBr_2F_2

M 209.8
Obt. by bromination of CH_2F_2. Fire-fighting agent; reagent for organic synth. Colourless, heavy non-flammable liq. Insol. H_2O. d_{15} 2.306 (2.288). Mp −110° (−141°). Bp 24.5° (23.2°). $T_{crit.}$ 198.2°.

▷ Mod. toxic; OES 860 mg m^{-3}. Dec. to toxic carbonyl halides if strongly heated in air. PA7525000.

Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)
Hamilton, J.M., *Adv. Fluorine Chem.*, 1963, **3**, 117.
Occupational Exposure Limits 1991, Health and Safety Executive, H.M.S.O., London, 1991, EH40/91.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1109.

CBr_2F_3N — IC-002305

Dibromo(trifluoromethyl)amine

N,N-Dibromo-1,1,1-trifluoromethanamine, 11Cl

[88453-18-3]

F_3CNBr_2

M 242.8
From CF_3NClBr + Br_2 or from $CF_2{=}NBr$ + CsF + Br_2. Pale yellow solid involatile at −75°. Dec. in sunlight to $F_3CN{=}NCF_3$. Mp −56°.

Zheng, Y.Y. *et al, Inorg. Chem.*, 1984, **23**, 518 (*synth, ms, ir, F-19 nmr*)
O'Brien, B.A. *et al, J. Am. Chem. Soc.*, 1984, **106**, 4266 (*synth*)

CBr_2O — IC-002306

Carbonyl bromide

Carbonic dibromide, 9Cl. Dibromoketone

[593-95-3]

$COBr_2$

M 187.8
Interatomic distances: Br—C 205, C=O 113 pm; angle: BrCBr 110°. Formed from CO + Br_2 or by oxidation of CBr_4. Commercially available. Colourless fuming liq. Rapidly hydrol. by H_2O to HBr + CO_2. d^{15} 2.52. Mp −80°. Bp 64-65°.

▷ Toxic, highly irritating.

Schumacher, H.-J. *et al, Ber.*, 1928, **61**, 1671 (*synth*)
Hopper, M.J. *et al, J. Chem. Phys.*, 1968, **48**, 3765 (*ir*)
Phillips, B.A. *et al*, Tet, 1973, **29**, 3309 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 110 (*rev, bibl*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 472, 550.

CBr_2S — IC-002307

Carbonothioic dibromide, 9Cl

Thiocarbonyl dibromide

$Br_2C{=}S$

M 203.8
Formed from $Cl_2C{=}S$ + BBr_3. Deep-red liq. with penetrating smell. Slowly dimerises at 20°. Bp 47°.

Dimer: see *2,2,4,4-Tetrabromo-1,3-dithietane*, *IC-002846*
Steudel, R., *Z. Anorg. Allg. Chem.*, 1968, **361**, 180 (*ir, raman, ms*)
Diderrich, G. *et al, Chem. Ber.*, 1976, **109**, 3432 (*synth*)

CBr_2Zr_2 — IC-002308

Zirconium bromide carbide (Zr_2Br_2C), 11Cl

Dizirconium dibromide carbide

[99665-58-4]

Zr_2Br_2C

M 354.2
Carbide atoms are in trigonal antiprismatic holes between the Zr layers in the 1T structure of ZrBr (Br—Zr—Zr—Br). Synth. by heating $ZrCl_4$, Zr and graphite in stoichiometric amounts in sealed Ta tubes at 950° for 10 days. Red-brown solid.

Hwu, S.J. *et al, Inorg. Chem.*, 1986, **25**, 283 (*synth, cryst struct, pe*)

CBr_3Cl — IC-002309

Tribromochloromethane, 9Cl, 8Cl

R 10B3

[594-15-0]

CBr_3Cl

M 287.1
Light-sensitive component in photographic emulsion for coloured printout images. d_4^{15} 2.71. Mp 55°. Bp 160°. Dec. evolving Br_2 on exp. to light.

Lecomte, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1937, **204**, 1927 (*synth, ir, raman*)
Hamilton, J.M., *Adv. Fluorine Chem.*, 1963, **3**, 117.
Delwaulle, H.L. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1195 (*raman*)

CBr_3F — IC-002310

Tribromofluoromethane, 9Cl, 8Cl

Fluorocarbon 11B3. Halon 1103

[353-54-8]

CBr_3F

M 270.7
Fire-extinguishing agent. d_{20} 2.76. Mp −73.6°. Bp 107.95°.

Desirant, Y., *Bull. Soc. Chim. Belg.*, 1958, **67**, 676 (*synth*)
Haszeldine, R.N. *et al, J. Chem. Soc.*, 1959, 13 (*synth*)
Tsyashchenko, Yu.P. *et al, Zh. Prikl. Spektrosk.*, 1972, **16**, 294; *CA*, **77**, 11913r (*cryst*)
Lo, E.S. *et al, J. Org. Chem.*, 1973, **38**, 907 (*nmr, ir*)

$CBr_3OPd^{\ominus}$ — IC-002311

Tribromocarbonylpalladate(1−), 9Cl

Carbonyltribromopalladate(1−)

[66213-28-3]

$[PdBr_3CO]^{\ominus}$

M 374.1 (ion)
Ir ν_{CO} 2120 cm^{-1} (CH_2Cl_2).
K salt: Yellow-green solid.
Tetrabutylammonium salt: [66213-29-4].
Catalyses carbonylation of aromatic nitro compounds.
Red cryst. (Et_2O). Mp 120° dec.

Kutyukov, G.G. *et al, Zh. Neorg. Khim.*, 1968, **13**, 1542; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 809 (*synth*)
Browning, J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, pmr, raman*)
Tietz, H. *et al, Z. Chem.*, 1980, **20**, 295 (*use*)
Andreini, B.P. *et al, J. Organomet. Chem.*, 1988, **354**, 369 (*struct, ir*)

$CBr_3OPt^{\ominus}$ — IC-002312

Tribromocarbonylplatinate(1−)

[66197-25-9]

$[PtBr_3(CO)]^{\ominus}$

M 462.8 (ion)
Ir ν_{CO} 2089 cm^{-1} (CH_2Cl_2).
K salt: Yellow-orange cryst. Mp 100° dec.
Tetrapropylammonium salt: Yellow cryst. (Me_2CO/Et_2O). Mp 121°.

Malatesta, L. *et al, Gazz. Chim. Ital.*, 1960, **90**, 1505 (*synth*)
Browning, J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, nmr, raman*)
Andreini, B.P. *et al, J. Organomet. Chem.*, 1988, **354**, 357 (*ir*)

CBr_3ORh — IC-002313

Tribromocarbonylrhodium, 8Cl

[27857-59-6]

$RhBr_3CO$

M 370.6
Dark-red cryst. Ir ν_{CO} 2110 cm^{-1} (KBr).

Colton, R. *et al, Aust. J. Chem.*, 1970, **23**, 1351 (*synth, ir*)

CBr_3ORu — IC-002314

Tribromocarbonylruthenium(*III*), 8Cl

[32073-81-7]

$Ru(CO)Br_3$

M 368.7

Struct. unknown, but certainly polymeric. Synth. in an impure form, from reaction between $RuBr_3$, MeOH and CO. Deep-red. Sol. MeOH. Ir ν_{CO} 2032 cm^{-1} (MeOH). Compd. not isol. pure.

Colton, R. et al, Aust. J. Chem., 1971, 24, 903 (ir, synth)

IC-002315

CBr_4

Carbon tetrabromide

Tetrabromomethane, 9CI

[558-13-4]

CBr_4

M 331.6

Sol. EtOH, Et_2O, $CHCl_3$, insol. H_2O. $d_4^{99.5}$ 2.961. Mp 90-91°. Mp 94.3° (dimorphic). Bp_{50} 102°. $n_D^{99.5}$ 1.5942.

▷ Toxic vapour, TLV 1.4. FG4725000.

Wallach, O., Justus Liebigs Ann. Chem., 1893, 275, 149 (synth)
Kendall, J. et al, J. Am. Chem. Soc., 1923, 45, 973 (synth)
Schaum, K., Justus Liebigs Ann. Chem., 1928, 462, 207 (synth)
Nonez, P.G. et al, CA, 1936, 30, 5556 (synth)
Bretherick, L., Handbook of Reactive Chemical Hazards, 2nd Ed., Butterworths, London and Boston, 1979, 278.
Sax, N.I., Dangerous Properties of Industrial Materials, 5th Ed., Van Nostrand-Reinhold, 1979, 471.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 231.

IC-002316

$CBr_5IrO^{2\ominus}$

Pentabromocarbonyliridate(2 –), 9CI

$[Ir(CO)Br_5]^{2\ominus}$

M 619.7 (ion)

Di-K salt: [15928-66-2].
CBr_5IrK_2O M 697.9
Pink cryst. (H_2O)

Di-Cs salt: [18532-80-4].
CBr_5Cs_2IrO M 885.5
Orange-brown solid. Sl. sol. H_2O. Ir ν_{CO} 2038 cm^{-1} (nujol).

Bis-Et_4N salt: [38478-21-6].
Ir ν_{CO} 2033 cm^{-1} ($MeNO_2$).

Malatesta, L. et al, J. Chem. Soc., 1964, 961 (synth)
Bonamico, M. et al, Ric. Sci., Parte 2: Sez. A, 1964, 7, 613; CA, 63, 12437g (struct)
Cleare, M.J. et al, J. Chem. Soc. A, 1969, 372; 1970, 2788 (synth, ir, raman)
Forster, D. et al, Synth. React. Inorg. Metal-Org. Chem., 1971, 1, 223 (synth, ir)
Cleare, M.J. et al, Spectrochim. Acta, Part A, 1972, 28, 2019 (ir, raman)

IC-002317

$CBr_5ORb^{2\ominus}$

Pentabromocarbonylrhodate(2 –), 10CI

[44028-64-8]

$[RhBr_5CO]^{2\ominus}$ (C_{4v})

M 536.4 (ion)

Catalyst for the reduction of Fe^{3+} to Fe^{2+}.

Di-Cs salt: [22594-89-4].
CBr_5Cs_2ORh M 796.2
Orange-red cryst. Ir ν_{CO} 2067 cm^{-1} (nujol).

Bis-Et_4N salt: [24396-67-6].
Orange cryst. Ir ν_{CO} 2070 cm^{-1} (nujol).

Forster, D., Inorg. Chem., 1969, 8, 2554 (synth, ir)
Cleare, M.J. et al, J. Chem. Soc. A, 1969, 372 (synth, ir, raman)
Colton, R. et al, Aust. J. Chem., 1970, 23, 1351 (synth, ir)
Dalton, D.J. et al, Inorg. Nucl. Chem. Lett., 1970, 6, 15 (struct)
Cleare, M.J. et al, Spectrochim. Acta, Part A, 1972, 28, 2019 (raman, ir)
James, B.R. et al, Can. J. Chem., 1977, 55, 567 (use)

IC-002318

$CBr_5ORu^{2\ominus}$

Pentabromocarbonylruthenate(2 –), 9CI, 8CI

$[Ru(CO)Br_5]^{2\ominus}$

M 528.6 (ion)

Deep red soln. in MeOH. Ir ν_{CO} 2038 cm^{-1} (aq. HBr). Paramagnetic.

Di-Cs salt: [30191-89-0].
Synth. by adding CsBr to a soln. obt. by passing CO through $RuBr_3$ in MeOH. Red cryst; dark blue cryst. form believed to be contaminated with Ru(*II*). Ir ν_{CO} 1996; ν_{RuC} 487; ν_{RuBr} 235, 185 cm^{-1}.

Cleare, M.J. et al, J. Chem. Soc. A, 1970, 2788 (synth, ir)
Colton, R. et al, Aust. J. Chem., 1971, 24, 903 (synth, ir)
Cleare, M.J. et al, Spectrochim. Acta, Part A, 1972, 28, 2019 (synth, ir, raman)

IC-002319

$CCaN_2$

Calcium cyanamide

Calcium carbimide, INN. Calcium carbodiimide. Cyanamide, calcium salt (1:1), 8CI. Aero cyanamid. Alzodef. CCC. Nitrolime. Nitrogen lime. Lime-nitrogen

[156-62-7]

$Ca(NCN)$

M 80.1

Manuf. from: CaC_2 + N_2 at 1000°. Synth. from CaO + $(H_2NCN)_2$ at 800°; $CaCO_3$ + HCN at 700 - 850°; $CaCl_2$ + NaCN at 600°. Commercially available. Anthelmintic used as fertiliser, herbicide, defoliant, pesticide, in manuf. of iron, cyanamide, cyanoguanidine and melamine. Colourless hexagonal cryst. Moisture sensitive: evolves NH_3 with water vapour. Dec. in H_2O. Mp *ca.* 1340°. Also known as cyanamide, although this name strictly applies to Cyanamide, IC-002509. ΔH_f° −348.3 kJ mol^{-1}, ΔG_f° −303 kJ mol^{-1}.

▷ Mod. toxic, flammable. GS6000000.

Compound with citric acid 2:1: [8013-88-5]. *Dipsan. Abstem. Temposil*
Commercially available. Used in treatment of alcoholism; inhibits aldehyde dehydrogenase.

Sokhorskov, B.I. et al, Opt. Spektrosk., 1959, 7, 663 (ir)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, 83, 962 (rev, bibl)
Vannerberg, N.G., Acta Chem. Scand., 1962, 16, 2263 (cryst struct)
Hoeger, R., Ullmanns Encykl. Tech. Chem., 4. Aufl., 1975, 9, 15 (rev)
Hoeger, H., Encycl. Chem. Process. Des., 1978, 6, 36 (rev)
Peachey, J.E. et al, J. Clin. Psychopharmacol., 1981, 1, 21 (pharmacol)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 1558 (therap)
Brien, J.F. et al, Drug. Metab. Rev., 1983, 14, 113 (pharmacol)
Sax, N.I. et al, Dangerous Properties of Industrial Materials, 7th Ed., Van Nostrand-Reinhold, 1989, 679 (haz, tox)

IC-002320

$CCaO_3$

Calcium carbonate ($CaCO_3$), USAN, BAN

Carbonic acid, calcium salt, 8CI. Limestone. Chalk

[471-34-1]

$CaCO_3$

M 100.0

Crude $CaCO_3$ is obt. by direct processing of mineral ores. Pure $CaCO_3$ prepd. by calcination of crude $CaCO_3$ followed by recombination of CaO and CO_2. Ultrapure $CaCO_3$ prepd. by treatment of aq. solns. of $CaCl_2$ with $[NH_4]_2CO_3$ and aq. NH_3. Commercially available. Road aggregate and building material. Raw material for quick lime (CaO) and slaked lime ($Ca(OH)_2$) production. Also used in manuf. of Portland cement. Used in paper manuf. to add brightness, opacity, ink receptivity and smoothness. Used as filler in cosmetics, rubbers, latex, paints and enamels. Also used in toothpastes and as an antacid. Component of Camalox, Titralac. Dec. on heating with loss of CO_2. Dissolves in acids → corresp. calcium salt. Colourless cryst. Hygroscopic. Prac. insol. H_2O. Mp 1339° (at 1.35 atm).

Mineral-form [14791-73-2]

Aragonite

Trimorphous with calcite and vaterite. Widespread occurrence. Cryst., wide variety of colours conferred by impurities. Often fluorescent. Prac. insol. H_2O (1.5 × 10^{-3} g per 100 cm^3 at 25°). ΔH_f° −1207.1 kJ mol^{-1}; ΔG_f° −1127.8 kJ mol^{-1}; S° 88.7 J K^{-1} mol^{-1}. Transforms to calcite at 520°.

Mineral-form [13397-26-7]

Calcite, Iceland spar

Widespread occurrence: chief constit. of limestones and marbles. Cryst. form extremely varied. Colourless when pure. Impurities give grey, yellow, brown, red, green, blue and black colouration. Often fluorescent and phosphorescent under u.v. Prac. insol. H_2O (1.4 × 10^{-3} g per 100 cm^3 at 25°). ΔH_f° −1206.9 kJ mol^{-1}; ΔG_f° −1128.8 kJ mol^{-1}; S° 92.9 J K^{-1} mol^{-1}

Mineral-form [13701-58-1]

Vaterite

Occurs in hydrogel pseudomorphs at Ballcraigy, N. Ireland and Hatrurim Formation, Israel. Colourless, fibrous cryst.

Swanson, H.E. et al, Natl. Bur. Std. Circ. 539, 1954, 3, 53 (aragonite, cryst struct)
McConnell, Mineral. Mag., 1960, 32, 535 (vaterite, cryst struct)
Graf, D.L., Am. Mineral., 1961, 46, 1283 (calcite, cryst struct)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, 83, 861 (rev, bibl)
Ross, S.D. et al, Spectrochim. Acta, 1964, 20, 781 (ir)
Porto, S.P.S. et al, Phys. Rev., 1966, 147, 608 (raman)
Goldsmith, J.A. et al, Spectrochim. Acta, 1966, 22, 1069 (ir)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, 1, 103 (uses)
Langille, D.B. et al, J. Phys. Chem. Solids, 1977, 38, 1149 (ir, raman)
Kummer, P. et al, Handb. Füllers Reinf. Plast., 1978, 81 (rev, uses)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 4, 427; 11, 698 (rev, uses)
Brown, A. et al, J. Geol. Educ., 1980, 28, 92 (rev, ir)
Arai, Y. et al, Gypsum Lime, 1981, 170, 25 (rev, struct)
Orwoll, E.S. et al, Ann. Intern. Med., 1982, 97, 242 (pharmacol)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 682.
Volz, F.E., Appl. Opt., 1983, 22, 1842 (ir, specular reflectance)
Sax, N.I. et al, Dangerous Properties of Industrial Materials, 7th Ed., Van Nostrand-Reinhold, 1989, 677.

IC-002321

$CCa_2O_3Si_2$

Scawtite

Calcium carbonate silicate ($Ca_7(CO_3)(Si_6O_{18})$)

[12166-06-2]

$Ca_7(Si_6O_{18})(CO_3)\cdot 2H_2O$

M 797.0

Unbranched, monocyclosilicate with $6SiO_4$ tetrahedra per ring. Mineral, occurs in China. Colourless transparent cryst.

[1319-55-7, 51681-13-1]

Murdoch, J., Am. Mineral., 1955, 40, 505.
Pluth, J.J. et al, Acta Crystallogr., Sect. B, 1973, 29, 73 (cryst struct)
Povarennykh, A.S. et al, Mineral. Zh., 1979, 1, 3; CA, 93, 171111 (ir)
Stevula, L. et al, Silikaty (Prague), 1982, 26, 137 (synth)

IC-002322

$CCa_{10}O_{27}P_6$

Calcium carbonate phosphate ($Ca_{10}(CO_3)(PO_4)_6$)

Decacalcium carbonate hexaphosphate

$Ca_{10}(CO_3)(PO_4)_6$

M 1030.6

Composition v. variable, with structural cavities. Apatite hexagonal struct. Synth. from $CaHPO_4$ + $CaCO_3$; Ca acetate aq. + mixed $PO_4^{3\ominus}$-$CO_3^{2\ominus}$; Calcium hydroxide phosphate ($Ca_5(OH)(PO_4)_3$). IC-016091 + CO_2 at 900°; Calcium fluoride phosphate ($Ca_5F(PO_4)_3$). IC-016088 + $CaCO_3$.

Mineral-form [61027-80-3]

Carbonate apatite

Essentially the monohydrate. Apatite struct. type with hexagonal lattice. Found in Turkey and Tashkent, Israel, India and regions of USSR. In urinary calculi.

[12286-89-4]

Zapanta-LeGeros, R., Nature (London), 1965, 206, 403.
Simpson, D., Science (Washington, D.C.), 1965, 147, 501 (props)
Bonel, G., Ann. Chim. (Paris), 14th Ser., 1972, 7, 65, 127 (synth, props)
Santos, M. et al, Inorg. Chem., 1977, 16, 2131 (synth, ir)
Roux, P. et al, Bull. Mineral., 1978, 101, 448 (ir, props)
Elliott, J.C. et al, J. Appl. Crystallogr., 1980, 13, 618 (cryst struct)

IC-002323

$CCdO_3$

Cadmium carbonate ($CdCO_3$)

Carbonic acid, cadmium salt (1:1)

[513-78-0]

$CdCO_3$

M 172.4

Calcite struct. Synth. from $CdCl_2$ and $(NH_4)_2CO_3$ in aq. NH_3. Rhombohedral leaflets. Spar. sol. H_2O; sol. acid. Dec. to CdO and CO_2 at 310°.

▷ FF9120000.

Gmelin Handbook Inorg. Chem., Syst. No. 35, 1958, 544.
Graf, D.L. et al, Am. Mineral., 1961, 46, 1283 (powder struct)
Miranda, J. et al, J. Phys. (Paris), 1967, 28, 152 (ir)
Sterzel, W., Z. Anorg. Allg. Chem., 1969, 368, 308 (ir)
Joergensen, C.K. et al, Kgl. Dan. Vidensk. Selsk. Mats.-Fys. Medd., 1972, 38 (pe)
Haas, H. et al, J. Chem. Phys., 1973, 58, 3339 (Cd-111 nqr)
Brauer, G., Handbuch Präp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 1049 (synth)
Nolle, A., Z. Naturforsch., A, 1978, 33, 666 (Cd-113 nmr, solid)
Schrommer, L.R. et al, J. Solid State Chem., 1980, 76, 140 (powder struct, thermal anal)

IC-002324

[CCe]

Cerium carbides

Phases CeC, Ce_2C_3, CeC_2 reported.

Cerium carbide (Ce_2C_3) [12015-43-9]

Cerium sesquicarbide

Isostructural with Pu_2C_3. Silvery solid. Ox. state of C ~ 3.4. Dec. by H_2O affording largely ethyne at r.t; at 200°, mostly ethene but 25% C_3 hydrocarbons.

Cerium carbide (CeC_2) [12012-32-7]
Cerium dicarbide
C_2Ce M 164.1
Possesses CaC_2 struct. Converts low MW alcohols into mols. of higher mass. Treatment with CCl_4 in hot melt, affords ultrahard C. Red cryst. brassy yellow powder. Mp 2250°. $\alpha \rightarrow \beta$ transition at 1090°. Dec. by H_2O, principally to ethyne with ethene, ethane and other hydrocarbons. $\mu_{eff} = 2.19\mu_B$ ($\theta = 61°$); $T_N \sim 30K$.

Zachariasen, W.H. *Acta Crystallogr.*, 1952, **5**, 17 (*cryst struct, Ce_2C_3*)
Brewer, L. *et al, J. Electrochem. Soc.*, 1956, **103**, 38 (*synth, Ce_2C_3*)
Spedding, F.H. *et al, J. Am. Chem. Soc.*, 1958, **80**, 4499 (*struct, synth, Ce_2C_3*)
Vickery, R.C. *et al, J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, magnetism*)
Atoji, M., *J. Chem. Phys.*, 1961, **35**, 1950, 1960; 1967, **46**, 1891, 4148; 1980, **73**, 5190 (*struct, magnetism, nd, Ce_2C_3*)
Palenik, G.J. *et al, Inorg. Chem.*, 1962, **1**, 345 (*reaction, Ce_2C_3*)
Saari, E., *Ann. Acad. Sci. Fenn., Ser. A2*, 1974, 174 (*synth*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Jones, D.W. *et al, J. Solid State Chem.*, 1980, **62**, 172 (*cryst struct*)
Sakai, T. *et al, Mater. Res. Bull.*, 1980, **15**, 1001 (*magnetism*)
U.S. Pat., 4 352 787, (1982); *CA*, **97**, 200264 (*use*)
Kingcade, J.E. *et al, Inorg. Chem.*, 1984, **23**, 1334 (*ms*)
U.S. Pat., 4 533 775, (1985); *CA*, **104**, 188658 (*use*)
Karen, P. *et al, Collect. Czech. Chem. Commun.*, 1986, **51**, 1411 (*synth, hydrol*)

CClFO — IC-002325

Carbonyl chloride fluoride, 8Cl
Carbonic chloride fluoride, 11Cl, 9Cl
[353-49-1]

O=CClF

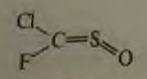
M 82.4
Synth. from CO + ClF. Colourless gas, stable at 20°, rapidly hydrol. Mp −148° Bp −47.2°, Bp −45°, −40°. T_{crit} 85°.

▷ Toxic. FG5425000.

Zanon, I. *et al, Spectrochim. Acta*, 1963, **19**, 301 (*uv*)
Kemmitt, R.D.W. *et al, Adv. Fluorine Chem.*, 1965, **4**, 142 (*rev*)
Christie, K.O. *et al, J. Org. Chem.*, 1965, **30**, 1639 (*synth*)
Gounelle, Y. *et al, Bull. Soc. Chim. Fr.*, 1968, 4835 (*ir*)
Siegemund, G., *Angew. Chem., Int. Ed. Engl.*, 1973, **12**, 918 (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 223 (*synth*)
Glavas, S. *et al, J. Photochem.*, 1985, **31**, 21 (*synth*)

CClFOS — IC-002326

Carbonothioic chloride fluoride *S*-oxide
Chlorofluoromethylene sulfoxide, Chlorofluorosulfine
[63674-09-9]



(E)-form

M 114.5
Exists as mixture of (E) and (Z) isomers. Unstable gas.

[63674-10-2]

Sander, W. *et al, Spectrochim. Acta, Part A*, 1986, **42**, 1281 (*synth, matrix ir*)
Henn, R. *et al, Chem. Ber.*, 1987, **120**, 1499 (*synth, ms, pe, matrix ir*)

CClFS — IC-002327

Thiocarbonyl chloride fluoride, 8Cl
Carbonothioic chloride fluoride, 11Cl, 9Cl, Thiocarbonyl chlorofluoride
[1495-18-7]

S=CClF

M 98.5
Yellow gas. Bp 9° (6-7°). Slowly hydrol. by H_2O.

Yarovenko, N.N. *et al, Zh. Obshch. Khim.*, 1959, **29**, 3792; *CA*, **54**, 19479e (*synth*)
Middleton, W.J. *et al, J. Org. Chem.*, 1965, **30**, 1375 (*synth, nmr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 643 (*synth*)

CClF$_2$N — IC-002328

***N*-Chlorodifluoroformimide**
N-Chlorodifluoromethanimine, 9Cl
[28245-33-2]

F_2C=NCl

M 99.4
Interatomic distances: F—C 130.0, C—N 125.4, N—Cl 170.0 pm; angle: FCN 126.2°. Formed from $ClCF_2NCl_2$ + Hg. Colourless gas, involatile at −125°. Bp 5°.

Young, D.E. *et al, J. Chem. Soc., Chem. Commun.*, 1970, 395 (*synth, ir, ms, F-19 nmr*)
Zheng, Y.Y. *et al, J. Org. Chem.*, 1983, **48**, 4844 (*synth, reactions*)
Groner, P. *et al, J. Mol. Struct.*, 1987, **160**, 37 (*microwave*)

CClF$_2$NO — IC-002329

Difluorocarbamic chloride, 9Cl
Difluorocarbamoyl chloride
[16847-30-6]

ClC(O)NF_2

M 115.4
Formed from F_2NCOF + $AlCl_3$. Colourless gas, stable to 180°. Sol. org. solvs. Bp −5°.

Fraser, G.W. *et al, Inorg. Chem.*, 1967, **6**, 1711 (*synth, ir, F-19 nmr*)
Wright, K.W. *et al, Inorg. Chem.*, 1973, **12**, 77 (*synth, reactions*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 135 (*rev, bibl*)

CClF$_2$NOS — IC-002330

(Chlorocarbonyl)imidosulfurous difluoride
[53654-97-0]

ClC(O)N=SF_2

M 147.5
Synth. from $[SF_2NCO][AsF_6]$ + NOCl. Not isol. in pure form. Isomerises to (Fluorocarbonyl)imidosulfurous chloride fluoride, IC-002331.

Mews, R.J., *J. Fluorine Chem.*, 1974, **4**, 445 (*synth, ir, F-19 nmr*)

CClF$_2$NOS — IC-002331

(Fluorocarbonyl)imidosulfurous chloride fluoride
[53654-99-2]

FC(O)N=SClF

M 147.5

Formed by isomerisation of (Chlorocarbonyl) imidosulfurous difluoride, IC-002330. Colourless liq., dec. at 25° to $COFNSCl_2$ + $COFNSF_2$. Forms 1:1 adduct with AsF_5.

Mews, R.J., *J. Fluorine Chem.*, 1974, **4**, 445 (*synth, ir, F-19 nmr*)

CClF$_2$NO$_3$S$_2$ — IC-002332

***N,N*-Bis(fluorosulfonyl)carbamoyl chloride, 8Cl**
N-(Chloroformyl)bis(fluorosulfonyl)amine
[7221-14-9]

$(FSO_2)_2$NCOCl

M 243.5
Synth. from Chloroimidodisulfuryl fluoride, IC-016342 + CO at 50°. Colourless liq., readily hydrol. to $HN(SO_2F)_2$. Bp_{31} 42°.

Ruff, J.K., *Inorg. Chem.*, 1966, **5**, 732 (*synth, ir, ms, F-19 nmr*)

CClF$_3$ — IC-002333

Chlorotrifluoromethane, 9Cl
Trifluoromethyl chloride. Fluorocarbon 13. Arcton 13. Freon 13
[75-72-9]

$CClF_3$

M 104.4
Fire extinguishing agent, low-temp. refrigerant, dielectric. Gas. Fp −181°. Bp −81.4°.

▷ Mod. toxic by inhalation. Production controlled by environmental legislation. Dec. to toxic carbonyl halides if strongly heated in air. PA6410000.

Haszeldine, R.N., *J. Chem. Soc.*, 1951, 584 (*synth*)
Hauptschein, M. *et al, J. Am. Chem. Soc.*, 1952, **74**, 1347 (*synth*)
Beattie, W.H., *Appl. Spectrosc.*, 1975, **29**, 334; *CA*, **83**, 124838n (*ms*)
de Marco, R.A. *et al, J. Magn. Reson.*, 1975, **18**, 522 (*cmr*)
Biedermann, S. *et al, J. Mol. Spectrosc.*, 1975, **56**, 367 (*ir*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 899.

CClF$_3$HgSe — IC-002334

Chloro(trifluoromethaneselenolato)mercury
Trifluoromethylselenylmercury chloride

$F_3CSeHgCl$

M 384.0
Part. disproportionates in soln. (e.g. MeOH) to $(F_3CSe)_2Hg$ and $HgCl_2$. From $(F_3CSe)_2Hg$ and $HgCl_2$. Pale yellow cryst. Readily sol. most org. solvs. Mp 175-177° (185-190°). Subl. 70° under vacuum.

Dale, J.W. *et al, J. Chem. Soc.*, 1958, 2939 (*synth*)
Birchall, T.J. *et al, Can. J. Chem.*, 1965, **43**, 1672 (*synth, Se-77 nmr*)
Clase, H.J. *et al, J. Chem. Soc.*, 1965, 940 (*synth, ir, raman*)

CClF$_3$O$_4$ — IC-002335

Trifluoromethyl perchlorate
Perchloric acid, trifluoromethyl ester, 9Cl
[52003-45-9]

F_3COClO_3

M 168.4
Synth. from CF_3I + $ClOClO_3$. Colourless gas, stable at r.t. Bp 9.3°.

Schack, C.J. *et al, Inorg. Chem.*, 1974, **13**, 2374 (*ir, raman*)
Schack, C.J. *et al, Inorg. Nucl. Chem. Lett.*, 1974, **10**, 449 (*synth*)

ClHgNS — IC-002336

Chloro(thiocyanato-*S*)mercury, 10Cl
Mercury(II) chloride thiocyanate
[26579-31-7]

ClHgSCN

M 294.1
Phototropic yellow solid. Insol. MeOH.

Takei, K., *Bull. Chem. Soc. Jpn.*, 1955, **28**, 408 (*synth, uv reflectance*)
Zhdanov, G.S. *et al, CA*, 1956, **50**, 16247 (*cryst struct*)
Tramisr, A., *J. Chim. Phys. Physt.-Chim. Biol.*, 1962, **59**, 232 (*ir*)
Gaizer, F. *et al, CA*, 1970, **72**, 137036 (*stability const*)
Belevantsev, V.I. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 511 (*stability const*)
Konovalov, L. *et al, Koord. Khim.*, 1986, **14**, 201 (*ir*)

ClClN$_2$O$_4$ — IC-002337

Chloroiododinitromethane, 9Cl
[40956-65-8]

$ClC(NO_2)_2$

M 266.3
▷ PA6405000.

Fridman, A.L. *et al, Khim.-Farm. Zh.*, 1976, **10**, 53; *CA*, **85**, 154480y (*synth, tox*)

CClN — IC-002338

Chlorine isocyanide
Isocyanogen chloride
[75754-69-7]

ClN≡C

M 61.4
Identified by photolysis of a matrix of ClCN, not isol.

Milligan, D.E. *et al, J. Chem. Phys.*, 1967, **47**, 278 (*uv, ir*)

CClN — IC-002339

Cyanogen chloride ((CN)Cl), 11Cl
Chlorine cyanide
[506-77-4]

ClC≡N ($C_{\infty v}$)

M 61.4
Interatomic distances: Cl—C 162.9, C≡N 116.0 pm. Synth. from NaCN + Cl_2 or HCN + Cl_2 or $(ClNCO)_3$ + Me_3SiCN. Military poison gas. Synthetic reagent. Commercially available. Colourless gas, readily trimerises to $(ClCN)_3$. Rapidly hydrol. by H_2O to CO_2 and cyanic acid. Stable up to 30°. V. sol. H_2O; many org. solvs. d_4^{12} 1.196, d^0 1.2. Fp −6°, Mp −5° Bp 13° (12.7°).

▷ Severe irritant, v. toxic; corrosive, poisonous fumes evolved on contact with H_2O or on heating; lachrymator, flammable. GT2275000.

Price, T. *et al, J. Soc. Chem. Ind., London*, 1920, **39**, 98T (*synth*)
Cook, R.P. *et al, J. Chem. Soc.*, 1935, 1001 (*synth, props*)
Inorg. Synth., 1946, **2**, 90 (*synth*)
King, G.W. *et al, J. Mol. Spectrosc.*, 1966, **21**, 353 (*struct*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 176; 1974, **4**, 110; 1980, **8**, 132.
Milligan, D.E. *et al*, *J. Chem. Phys.*, 1957, **47**, 278 (*ir, #*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 630 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1978, **D3**, 185 (*rev, bibl*)
Nachbaur, E. *et al*, *Monatsh. Chem.*, 1978, **109**, 1211 (*synth*)
Whiffen, D.H., *Spectrochim. Acta, Part A*, 1978, **34**, 1173 (*struct*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 279.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 987.

IC-002340

CCINO

Chlorine isocyanate

Chloroisocyanate

[13858-09-8]

Cl—N=C=O (C_s)

M 77.4

Has *trans*-stereochem. Interatomic distances: Cl—N 170.3, N—C 121.8, C—O 116.5 pm; angles: NCO 171°, ClNC 119°. Formed by pyrolysis of $(ClNCO)_3$ at 200°

Colourless liq. or gas, readily hydrol. Slowly dec. above −95°. Mp −98.5° Bp 1.6°.

Trimer: see *1,3,5-Trichloro-1,3,5-triazine-2,4,6(1H,3H,5H)-trione*, *IC-003539*

Nachbaur, E. *et al*, *Monatsh. Chem.*, 1966, **97**, 115 (*synth*)
Eysel, H.H. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **381**, 71 (*ir, raman*)
Hocking, W.H. *et al*, *J. Mol. Spectrosc.*, 1972, **42**, 547 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 137 (*bibl*)

IC-002341

$CClNO_3S$

Sulfuryl chloride isocyanate, 9CI

Chlorosulfonyl isocyanate. *N-Carbonylsulfonyl chloride*

[1189-71-5]

$ClSO_2NCO$

M 141.5

Synth. from ClCN + SO_3 at 130°. Versatile synthetic reagent. Most reactive known isocyanate. Also brings about aromatic chlorinations. Liq. which fumes in moist air forming CO_2 + H_2NS_2OH + HCl. d_4^{20} 1.626. Mp <−80°. Bp 106-107°, Bp 54-56°. n_D^{27} 1.4435. Stable to 300°.

▷ Reacts violently with H_2O. V. strong irritant.

Org. Synth., 1966, **46**, 23 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 117; 1979, **7**, 65; 1988, **13**, 80 (*use*)
Graf, R., *Angew. Chem., Int. Ed. Engl.*, 1968, **7**, 172 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 495.
Srinivasan, T.N. *et al*, *Synth. Commun.*, 1986, **16**, 543.
Dhar, D.N. *et al*, *Synthesis*, 1986, 437 (*rev*)
Kamai, A. *et al*, *Heterocycles*, 1987, **26**, 1051 (*rev*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 279.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 890.

CCINS

IC-002342

Thiocyanogen chloride

Chlorothiocyanate

[5961-98-8]

N≡CSCl

M 93.5

Synth. from $S_2(CN)_2$ + Cl_2 or $Pb(SCN)_2$ + Cl_2. Used in org. synth. Known only in soln. (golden-yellow). Slowly polym. at 20°.

Angus, A.B. *et al*, *J. Chem. Soc.*, 1958, 774 (*synth, str*)
Nelson, M.J. *et al*, *J. Chem. Soc.*, 1960, 604 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1978, **D6**, 174 (*rev, bibl*)

CCl_2F_2

IC-002343

Dichlorodifluoromethane, 9CI

Fluorocarbon 12. *Freon 12*. *Arcton 12*. *Genetron 12*

[75-71-8]

CCl_2F_2

M 120.9

Refrigerant, aerosol propellant, foam blowing agent, leak-detecting agent, low-temp. solv. Almost odourless gas. Fp −158°. Bp −29.8°, Bp_{7000} 42.4°.

▷ OES 4950 mg m^{-3}. Can react violently with Al or Mg. Dec. to toxic carbonyl halides if strongly heated in air. Production controlled by environmental legislation. PA8200000.

Henne, A.L., *Org. React. (N.Y.)*, 1944, **2**, 49 (*rev*)
Chait, E.M. *et al*, *Org. Mass Spectrom.*, 1969, **2**, 1135 (*ms*)
Abraham, R.J. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1973, 1027 (*nmr*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 277.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1143.

CCl_2F_2Se

IC-002344

Chlorodifluoromethaneselenenyl chloride, 9CI

[54393-40-7]

$F_2ClCSeCl$

M 199.8

Formed from $F_2C{=}Se$ + Cl_2 at −60°. Red liq. Bp_{50} 28°.

Haas, A. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **427**, 114 (*synth, ir, ms, F-19 nmr*)
Gombler, W., *J. Am. Chem. Soc.*, 1982, **104**, 6616 (*Se-77 nmr*)

$CCl_2F_3S_2^{\oplus}$

IC-002345

Dichloro(trifluoromethylthio)sulfonium(*IV*)(1+)

$[F_3CSSCl_2^{\oplus}]$

M 204.0 (ion)

Chloride:
$CCl_3F_3S_2$ M 239.4
Formed from F_3CSSCl + Cl_2 at −100°. Exists only as a yellow solid. Mp −40° dec.

Minkwitz, R. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **564**, 135 (*synth, raman*)

CCl_2F_5NOS

IC-002346

(*N*-Chlorochloroformimidoyl)pentafluorosulfur

$ClN{=}C(Cl)OSF_5$

M 239.9

Formed from $F_5SOCCl_2NCl_2$ + Hg as mixt. of *cis* and *trans*-forms.

cis-form

Colourless liq. Mp −77°. Bp 86°.

trans-form

Colourless liq. Mp −87°. Bp 86°.

Schmack, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 134 (*synth, F-19 nmr, ir, raman, ms*)

CCl_2NOP

IC-002347

Phosphorisocyanatidous dichloride, 9CI

Dichloroisocyanatophosphine.
Dichloroisocyanatophosphorus(III)

[1858-29-3]

$Cl_2PN{=}C{=}O$

M 143.8

Pungent liq. Bp 104°.

▷ Extremely reactive to protic nucleophiles.

Fluck, E., *Z. Naturforsch., B*, 1964, **19**, 869 (*P-31 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 629 (*rev, bibl*)
Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1965, **338**, 52.
Gertsyuk, N.N. *et al*, *Zh. Org. Khim.*, 1981, **17**, 1389; *J. Org. Chem. USSR (Engl. Transl.)*, 1981, **17**, 1233 (*synth, ir*)

CCl_2NOPS

IC-002348

Phosphor(isothiocyanatidic) dichloride, 9CI

Dichloroisothiocyanatooxophosphorus(V)

[1858-38-4]

$SCNP(O)Cl_2$

M 175.9

V. reactive liq. Bp_1 40°.

Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1965, **338**, 58 (*P-31 nmr*)
Schmitt, R. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **358**, 38 (*synth, ir, raman*)

CCl_2NO_2P

IC-002349

Phosphor(isocyanatidic)dichloride, 9CI, 8CI

[870-30-4]

$OCNP(O)Cl_2$

M 159.8

Reactive liq. with fishy odour. d_4^{15} 1.65. Bp 138-139°, Bp_5 19.7-20°. n_D^{15} 1.470.

Kirsanov, A.V., *Zh. Obshch. Khim.*, 1954, **24**, 1033; *J. Gen. Chem. USSR (Engl. Transl.)*, 1954, **24**, 1031 (*synth*)
Naumov, V.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, (*Engl. transl.* p. 188), 1973, **209**, 118 (*ed, struct*)
Egorov, Yu.P. *et al*, *Zh. Strukt. Khim.*, 1973, **14**, 240; *J. Struct. Chem. USSR (Engl. Transl.)*, 1973, **14**, 216 (*ir*)
Kisilenko, A.A. *et al*, *Zh. Prikl. Spektrosk.*, 1978, **28**, 480; *J. Appl. Spectrosc. USSR (Engl. Transl.)*, 1978, **28**, 333 (*ir*)
Dillon, K.B. *et al*, *Phosphorus Sulfur*, 1984, **19**, 299 (*P-31 nmr*)
Sosnovsky, G. *et al*, *J. Med. Chem.*, 1986, **29**, 2225 (*synth*)

CCl_2O

IC-002350

Carbonyl chloride

Carbonic dichloride, 11CI, 9CI. *Phosgene*. *Chloroformyl chloride*

[75-44-5]

$O{=}CCl_2$ (C_{2v})

M 98.9

Bond lengths; Cl—C 174.6, C—O 116.6 pm; angle ClCCl 111.3°. Used in synthesis, employed as war gas in WWI. Commercially available. Colourless gas with penetrating odour. Dec. to CO + Cl_2. Sol. org. solvs. d_4^0 1.419. Mp −128° (−118°). Bp 7.6°. T_{crit} 182°.

▷ V. highly toxic, TLV 0.4. Mixt. with K explodes on shock. SY5600000.

Robinson, G.W., *J. Chem. Phys.*, 1953, **21**, 174 (*struct*)
Rodd's Chem. Carbon Compd. (2nd Ed.), 1965, **Ic**, 279 (*bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 856; 1969, **2**, 328; 1972, **3**, 225; 1975, **5**, 532; 1979, **7**, 289 (*use*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 650.
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **17**, 416.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 280.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2767 (*haz*)

CCl_2OS

IC-002351

Chlorocarbonylsulfenyl chloride

(Chlorothio)formyl chloride

[2757-23-5]

ClSC(O)Cl

M 130.9

Interatomic distances: Cl—S 201.0, S—C 179.1, C=O 118.3, C—Cl 174.9 pm. Formed from CCl_3SCl + aq. H_2SO_4 at 45-50°. Commercially available. Colourless cryst. Bp 98°.

▷ Corrosive, lachrymator.

Netherlands Pat., 6 514 548, (1965); *CA*, 1966, **65**, 12112b (*synth*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 645 (*synth*)
Shen, Q. *et al*, *J. Mol. Struct.*, 1985, **128**, 41 (*ed, struct*)

CCl_2OS_3

IC-002352

Chloro chlorocarbonyl trisulfide

1-Chloro-3-(chlorocarbonyl)trisulfane. *(Chlorocarbonyl) trisulfanyl chloride*

[100244-94-8]

ClS—S—SC(O)Cl

M 195.1

Formed in low yield by thermolysis of $(ClCO)_2S_4$.

Schroll, A.L. *et al*, *J. Org. Chem.*, 1986, **51**, 1866 (*synth, pmr*)

CCl_2OS_4

IC-002353

Chloro chlorocarbonyl tetrasulfide

1-Chloro-4-(chlorocarbonyl)tetrasulfane

[100244-90-4]

ClSSSSC(O)Cl

M 227.1

Formed by thermolysis of bis(chlorocarbonyl)sulfanes, S_4 to S_8. Not isol.

Schroll, A.L. *et al*, *J. Org. Chem.*, 1986, **51**, 1866 (*synth*)

CCl_2S

IC-002354

Carbonothioic dichloride, 9CI

Thiophosgene, 8CI. *Thiocarbonyl chloride*

[463-71-8]

$S{=}CCl_2$ (C_{2v})

M 114.9

Interatomic distances: Cl—C 172.9, C=S 160.1 pm; angle: ClCCl 111.2°. Formed by Fe reduction of Cl_3CSCl; by $SnCl_2$ reduction of CCl_3SOCl. Reagent for synth. of

isothiocyanates and *N*-isothiocyanatoimines. Commercially available in glass ampoules. Fuming red liq. with acrid odour. Sl. sol. H_2O; sol. Et_2O. Slowly hydrol. by H_2O. d_{15} 1.509. Bp 73-76°. n_D^{20} 1.5442.

▷ Severe irritant; poison. XN2450000.

S-Oxide: [24768-49-8]. (*Dichloromethylene*)*sulfoxide*

CCl_2OS M 130.9

Synth. from CCl_2SOCl + $SnCl_2$ or CCl_4 + S or from $SCCl_2$ + F_3CCO_3H in CH_2Cl_2 at −5°. Colourless liq., slowly dec. at 20° to phosgene and sulfur. Bp_{25} 34-36°, Bp_{14} 30-31°.

▷ Corrosive, toxic.

Dimer: see *2,2,4,4-Tetrachloro-1,3-dithietane*, IC-002894

Helfrich, O.B. *et al*, *J. Am. Chem. Soc.*, 1921, **43**, 591 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 506 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **22**, 110 (*manuf*)
Farnworth, E.R. *et al*, *J. Mol. Spectrosc.*, 1973, **46**, 419 (*uv*)
Moule, D.C. *et al*, *J. Mol. Spectrosc.*, 1973, **48**, 336 (*struct*)
Magerlein, H. *et al*, *Synthesis*, 1974, 26 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 668.
Oka, T. *et al*, *J. Chem. Phys.*, 1975, **63**, 2414 (*ir*)
Carpenter, J.H. *et al*, *J. Chem. Soc., Faraday Trans. 1*, 1975, 1752 (*struct*)
Sharma, S., *Synthesis*, 1978, 803 (*rev*)
Field, L. *et al*, *J. Org. Chem.*, 1979, **44**, 2624 (*deriv*)
Eschwey, M. *et al*, *Chem. Ber.*, 1983, **116**, 1623 (*synth, ir, ms, S-oxide*)
Jenner, G. *et al*, *Tetrahedron Lett.*, 1985, **26**, 725 (*reactions, S-oxide*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3261 (*tox*)

CCl_2Se IC-002355

Carbonoselenoic dichloride

Selenocarbonyl dichloride. Selenophosgene

[80008-70-4]

$Cl_2C{=}Se$

M 161.8

Formed by pyrolysis of *cyclo*-$(CCl_2Se)_2$. Dark blue liq., stable only below −130°.

▷ V. toxic.

Gmelin Handbook Inorg. Chem., Syst. No. 14, 1978, **D6**, 251 (*bibl*)
Darmadi, A. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1261 (*synth, ms, uv, ir, raman*)
Iacos, M.E., *J. Phys. Chem. Ref. Data*, 1984, **13**, 1002 (*ir*)

CCl_2Zr_2 IC-002356

Zirconium carbide chloride (Zr_2CCl_2), 11Cl

Dizirconium carbide dichloride

[99665-57-3]

Zr_2Cl_2C

M 265.3

Isostructural with Zirconium bromide carbide (Zr_2Br_2C), IC-002308. Synth. by heating $ZrCl_4$, Zr and graphite in stoichiometric amounts in a sealed Ta tube at 950° for 10 days. Red-brown solid.

Hwu, S.J. *et al*, *Inorg. Chem.*, 1986, **25**, 283 (*synth, cryst struct, pe*)

CCl_3F IC-002357

Trichlorofluoromethane, 9Cl

Fluorocarbon 11. Freon 11. Arcton 11. Genetron 11

[75-69-4]

Cl_3CF

M 137.3

Refrigerant, foam blowing agent, aerosol propellant and dry cleaning agent. Liq. d_4^{17} 1.49. Bp 23.8°.

▷ Dec. to toxic carbonyl halides if strongly heated in the presence of air. Production controlled by environmental legislation. OES 5600 mg m^{-3}. PB6125000.

Ruff, O. *et al*, *Z. Anorg. Allg. Chem.*, 1931, **201**, 245; *CA*, **26**, 1250 (*synth*)
Christie, K.O. *et al*, *J. Org. Chem.*, 1964, **29**, 3007 (*synth*)
Emsley, J.W., *Mol. Phys.*, 1964, **11**, 437; *CA*, **66**, 60540 (*nmr*)
Gallant, R.W., *Hydrocarbon Process.*, 1968, **47**, 135; *CA*, **68**, 86738k (*props*)
Chait, E.M. *et al*, *Org. Mass Spectrom.*, 1969, **2**, 1135; *CA*, **72**, 48903k (*ms*)
Doucet, J. *et al*, *J. Chem. Phys.*, 1973, **58**, 3708 (*uv*)
v. Hamme, M.J. *et al*, *J. Fluorine Chem.*, 1977, **10**, 131 (*use*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 338.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3331.

CCl_3FS IC-002358

Dichlorofluoromethanesulfenyl chloride, 9Cl

Cl_2FCSCl

M 169.4

d_0^{20} 1.61. Bp 99.5-100.5°.

▷ Mod. toxic.

Petrov, K.A. *et al*, *Zh. Obshch. Khim.*, 1959, **29**, 3401; *CA*, **54**, 14102b (*synth*)
Sheppard, W.A. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 5106 (*synth, nmr, ir*)
Ham, N.S., *J. Am. Chem. Soc.*, 1961, **83**, 751 (*raman*)
Seel, F. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1967, **6**, 706 (*nmr*)

CCl_3FSe IC-002359

Dichlorofluoromethaneselenenyl chloride

[62247-74-9]

$FCCl_2SeCl$

M 216.3

Formed from CSe_2 + ClF/Cl_2. Red liq. Bp_{38} 51°.

Haas, A. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **427**, 114 (*synth, ir, ms, F-19 nmr*)

CCl_3F_2N IC-002360

***N,N*-Dichloro(chlorodifluoromethyl)amine**

[28245-34-3]

$ClCF_2NCl_2$

M 170.3

Formed from ClCN + ClF at 20°. Colourless liq., dec. slowly at 20° to Cl_2 + $F_2C{=}NCl$.

Young, D.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 385 (*synth, ir*)
Zheng, Y.Y. *et al*, *J. Org. Chem.*, 1983, **48**, 4844 (*synth, reactions*)

CCl_3N IC-002361

Chlorocarbonimidic dichloride, 9Cl

Chloroimidocarbonyl chloride, 8Cl. N-Chlorochloroformimidoyl chloride. N-Chloroisocyanide dichloride

[25240-91-9]

$Cl_2C{=}NCl$

M 132.3

Formed from $ClC{\equiv}N$ + Cl_2 at 60°. Colourless liq. Bp 87°. Slowly dec. in air. Strong chlorinating agent; adds to alkenes.

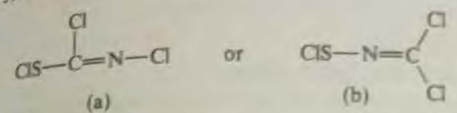
Hagemann, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 606 (*synth, ir*)
Burke, J.M. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 1649 (*raman, ir*)
Jupe, G. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1975, 925 (*ngr*)

CCl_3NS IC-002362

(Chlorothio)carbonimidic dichloride, 9Cl

(Chlorothio)imidocarbonyl chloride, 8Cl. Trichlorothiocyanate

[15999-70-9]



M 164.4

Struct. not resolved. Feher and Kauffmann favour (a) and Bacon and Kühle favour (b). Bacon also suggests a mixture of the two. Synth. from $S_2(CN)_2$ + excess Cl_2. Pungent orange liq., slowly dec. at 20°. Bp 154-155°, Bp_9 40-41°.

Kaufmann, H.P. *et al*, *Ber.*, 1924, **57**, 923 (*synth*)
Feher, F. *et al*, *Chem. Ber.*, 1958, **91**, 2523 (*synth, raman*)
Bacon, R.G.R. *et al*, *J. Chem. Soc.*, 1958, 764 (*synth, ir, struct*)
Kühle, E. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1967, **6**, 649 (*synth, ir, struct*)

$CCl_3OPd^{\ominus}$ IC-002363

Carbonyltrichloropalladate(1 −), 9Cl

Trichlorocarbonylpalladate(1 −)

[44252-60-0]

$[PdCl_3(CO)]^{\ominus}$

M 240.7 (ion)

Ir ν_{CO} 2132 cm^{-1} (CH_2Cl_2).

Diethylammonium salt: [75934-65-5].

Solid (heptane).

Tetrabutylammonium salt: [19508-35-1].

Catalyses carbonylation of aromatic nitro compounds. Orange cryst. (Me_2CO/Et_2O). Mp 95° dec.

Browning, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, raman, pmr*)
Tietz, H. *et al*, *Z. Chem.*, 1980, **20**, 295 (*use*)
Calderazzo, F. *et al*, *Inorg. Chem.*, 1981, **20**, 1310 (*synth, ir*)
Tietz, H. *et al*, *Z. Chem.*, 1985, **25**, 290 (*use*)
Andreini, B.P. *et al*, *J. Organomet. Chem.*, 1988, **354**, 369 (*struct, ir*)

$CCl_3OPt^{\ominus}$ IC-002364

Carbonyltrichloroplatinate(*II*)(1 −)

[21710-57-6]

$[PtCl_3(CO)]^{\ominus}$ (C_{3v})

M 329.4 (ion)

Catalyst/intermed. in reaction of NO and CO to produce N_2O and CO_2. Ir ν_{CO} 2118 cm^{-1} (H_2O), 2098 cm^{-1} (CH_2Cl_2), 2082 cm^{-1} (KBr).

Tetrabutylammonium salt: [34964-16-4].

Pale yellow cryst.

(2,2′-Bipyridine-N,N′)carbonylchloroplatinum(1 +) salt: [33679-79-7].

$C_{23}H_{24}Cl_3N_2O_3P_2Pt_2$ M 744.1

Yellow, moisture-sensitive solid.

Malatesta, L. *et al*, *Gazz. Chim. Ital.*, 1960, **90**, 1305 (*synth, props*)
Spaulding, L. *et al*, *Inorg. Chem.*, 1972, **11**, 2092 (*synth, ir*)
Pietropaolo, R. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 369 (*reactions*)
Cherwinski, W.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1156 (*ir*)
Russell, D.R. *et al*, *J. Organomet. Chem.*, 1976, **104**, 387 (*struct*)
Calderazzo, F. *et al*, *Inorg. Chem.*, 1981, **20**, 1310 (*ir*)
Sun, K.S. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 6744 (*synth, ir, props*)
Sun, K.S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 289 (*use, ir, uv*)
Andreini, B.P. *et al*, *J. Organomet. Chem.*, 1988, **354**, 357 (*ir*)

CCl_3ORh IC-002365

Carbonyltrichlororhodium, 8Cl

Trichlorocarbonylrhodium

[27857-62-1]

$RhCl_3CO$

M 237.2

Unstable when exposed to the atm. Characterised spectroscopically. Ir ν_{CO} 2135 cm^{-1} (KBr).

Colton, R. *et al*, *Aust. J. Chem.*, 1970, **23**, 1351 (*synth, ir*)

CCl_3ORu IC-002366

Carbonyltrichlororuthenium(*III*), 9Cl, 8Cl

[32073-80-6]

$Ru(CO)Cl_3$

M 235.4

Synth. by evaporating a soln. formed by treating $RuCl_3.xH_2O$ with boiling HCOOH/HCl mixt. Deep-red solid (impure, possibly contaminated with $RuCl_3$). Sol. MeOH, EtOH. Ir ν_{CO} 2045 or 2044 cm^{-1} (EtOH). Compd. not isol. pure because of ready reduction to ruthenium(*II*).

Manchot, W. *et al*, *Chem. Ber.*, 1924, **57**, 2130 (*synth*)
Colton, R. *et al*, *Aust. J. Chem.*, 1971, **24**, 903 (*synth, ir*)
Bersh, M.L. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 3763 (*synth, ir*)

CCl_4 IC-002367

Carbon tetrachloride

Tetrachloromethane, 9Cl. Perchloromethane. R10. F10

[56-23-5]

CCl_4

M 153.8

Solv. for org. compds., formerly used in fire extinguishers, formerly dry-cleaning solv., formerly used as anthelmintic. Grain fumigant. Used in manuf. of chlorofluoromethanes. Chlorinating agent. Sol. EtOH, Et_2O, prac. insol. H_2O. d_4^{20} 1.632. Bp 76.74°. Freezes to trimorphous solid having Mps. −28.6°, −23.8° and −21.2°. n_D^{20} 1.4631.

▷ Highly toxic by inhalation and skin contact, OES 65 mg m^{-3}. Dec. to highly toxic $COCl_2$ if strongly heated in the presence of air. Production controlled by environmental legislation. FG4900000.

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 69
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 705, 707 (*synth, props*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 767

Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 231.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 714.

IC-002368

CCl_4F_5NOS

[Dichloro(dichloroamino)methanolato-*O*]pentafluorosulfur, 9Cl

N-Dichlorodichloropentafluorosulfoxymethylamine

[106735-58-4]

$Cl_2NCCl_2OSF_5$

M 310.8
Formed from $F_5SOCl + Cl_2C{=}NCl$. Colourless liq. dec. in presence of Hg. Mp −39°.

Schmuck, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 134 (*synth, F-19 nmr, N-14 nmr, ir, ms*)

IC-002369

$CCl_5IrO^{2\ominus}$

Carbonylpentachloroiridate(2−), 9Cl

$[Ir(CO)Cl_5]^{2\ominus}$

M 397.4 (ion)
Di-K salt: [53779-01-4].
CCl_4IrK_2O M 475.6
Pink cryst. (EtOH/Et_2O). V. sol. H_2O.
Di-Cs salt: [15380-15-1].
CCl_4Cs_2IrO M 663.3
Pale-orange solid. Sl. sol. H_2O. Ir ν_{CO} 2070 cm^{-1} (nujol).
Bis-Et_4N salt: [38478-19-2].
Ir ν_{CO} 2039 cm^{-1} ($MeNO_2$).

Malatesta, L. *et al*, *J. Chem. Soc.*, 1964, 961 (*synth*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372; 1970, 2788 (*synth, ir, raman*)
Forster, D. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 221 (*synth, ir*)
Cleare, M.J. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 2019 (*ir, raman*)

IC-002370

$CCl_4NOsS^{2\ominus}$

Pentachloro(thiocyanato)osmate(*IV*)(2−)

$[OsCl_5(SCN)]^{2\ominus}$

M 425.5 (ion)
Synth. by oxidation of $[OsCl_4I]^{2\ominus}$ with $(SCN)_2$ in CH_2Cl_2. The isomers are separated by ion exchange chromatography and isolated as tetrabutylammonium salts.
Thiocyanato-N-form [94643-65-9]
Thiocyanato-S-form [94643-67-1]

Preetz, W. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **516**, 159 (*synth, ir, uv*)

IC-002371

$CCl_5OOs^{3\ominus}$

Carbonylpentachloroosmate(3−), 8Cl

$[Os(CO)Cl_5]^{3\ominus}$

M 395.4 (ion)
Tri-Cs salt: [17568-67-1].
CCl_4Cs_3OOs M 794.1
Orange cryst.

Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir*)

$CCl_5OOs^{2\ominus}$

IC-002372

Carbonylpentachloroosmate(2−), 9Cl

Pentachlorocarbonylosmate(2−)

$[Os(CO)Cl_5]^{2\ominus}$

M 395.4 (ion)
Di-Cs salt: [56027-95-3].
CCl_4Cs_2OOs M 661.2
Orange solid.

Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1970, 2788 (*synth, ir*)
Cleare, M.J. *et al*, *Spectrochim. Acta, Part A*, 1971, **28**, 2019 (*ir*)

$CCl_5OPt^{\ominus}$

IC-002373

Carbonylpentachloroplatinate(1−)

$[Pt(CO)Cl_5]^{\ominus}$

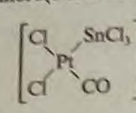
M 400.3 (ion)
Possible chlorination catalyst.
Diisopropylammonium salt: Yellow-orange solid. Loses Cl_2 in soln. Dec. by H_2O. Ir ν_{CO} 2191 cm^{-1}.

Crocker, C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 1056.
Dell'Amico, D.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 2257.
Andreini, B.P. *et al*, *J. Organomet. Chem.*, 1988, **354**, 357 (*cmr*)

$CCl_5OPtSn^{\ominus}$

IC-002374

Carbonyldichloro(trichlorostannyl)platinate(1−), 11Cl



cis-form

M 519.0 (ion)

cis-form

Tetrabutylammonium salt: [103303-84-0].
$C_{17}H_{36}Cl_5NOPtSn$ M 761.5
Yellow-orange cryst. (CH_2Cl_2/Et_2O).

Herbert, I.R. *et al*, *Inorg. Chim. Acta*, 1986, **112**, 29 (*synth, cmr, Sn-119 nmr, Pt-195 nmr*)

$CCl_5ORh^{2\ominus}$

IC-002375

Carbonylpentachlororhodate(2−), 9Cl

Pentachlorocarbonylrhodate(2−)

$[RhCl_5CO]^{2\ominus}$ (C_{4v})

M 308.1 (ion)
Di-Cs salt: [22594-88-3].
Orange cryst. Ir ν_{CO} 2117 cm^{-1} (nujol).
Bis-Me_4N salt: [24596-66-5].
Orange solid. Ir ν_{CO} ~2090br cm^{-1} (nujol).
Bis-Et_4N salt: [24596-65-4].
Orange cryst. Ir ν_{CO} ~2070br cm^{-1} (nujol).

Forster, D., *Inorg. Chem.*, 1969, **8**, 2556 (*synth, ir*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Stanko, J.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 1100 (*synth, ir*)
Colton, R. *et al*, *Aust. J. Chem.*, 1970, **23**, 1351 (*synth, ir*)
Dahm, D.J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 15 (*struct*)
Cleare, M.J. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 2019 (*ir, raman*)

$CCl_5ORu^{2\ominus}$

IC-002376

Carbonylpentachlororuthenate(*III*)(2−), 8Cl

[51418-48-5]

$[Ru(CO)Cl_5]^{2\ominus}$

M 306.3 (ion)
Paramagnetic. Soln. synth. either by passing CO into a soln. (HCl or MeOH) of $RuCl_3.xH_2O$ or $[RuCl_5(OH_2)]^{2\ominus}$, or by heating $RuCl_3.xH_2O$ with a mixt.of HCl/HCOOH. Invaluable synthetic reagent in alcoholic soln., for Ru(*III*) complexes, or on reduction (HCOOH/HCl; prolonged heating) for Ru(*II*) complexes. Blood red soln. in MeOH or H_2O. Ir ν_{CO} 2055 cm^{-1} (aq. HCl).
Di-K salt: [66115-12-6].
CCl_5K_2ORu M 384.5
Synth. by treating $K_2[RuCl_5(OH_2)]$ with boiling ethanolic HCl. Brick-red cryst. + H_2O (HCl aq.). μ_{eff} = 1.87μ_B; Ir ν_{CO} 1928, 1912, ν_{RuCl} 348, 310 cm^{-1}.
Di-Cs salt:
CCl_5Cs_2ORu M 572.1
Synth. by adding CsCl to blood red soln. Red solid. μ_{eff} = 1.72μ_B; Ir ν_{CO} 2030, ν_{RuCl_5} 336, 319, ν_{RuCl} 312, ν_{RuC} 480 cm^{-1}.
Di-Ammonium salt: Prep. by adding $[NH_4]Cl$ to blood-red soln. Red salt.
Bis-Benzyltriphenylphosphonium salt: Cryst. Ru—Cl 237.4, 248.1 pm.

Manchot, W. *et al*, *Ber.*, 1924, **57**, 2130 (*synth*)
Chatt, J. *et al*, *J. Chem. Soc.*, 1964, 3466 (*reactions*)
Halpern, J. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 5142 (*synth, uv*)
Stephenson, T.A. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 945 (*reactions*)
Bruce, M.I. *et al*, *J. Chem. Soc. A*, 1967, 1238 (*reactions*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372; 1970, 2788 (*synth, ir, raman, magnetism*)
Stanko, J.A. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 5580 (*cryst struct*)
Colton, R. *et al*, *Aust. J. Chem.*, 1971, **24**, 903 (*synth, ir*)
Collman, J.P. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 1788 (*reactions*)
Cleare, M.J. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 2019 (*ir, raman*)
Fergusson, J.E. *et al*, *Aust. J. Chem.*, 1978, **31**, 497 (*synth, ir*)
Gould, R.O. *et al*, *J. Chem. Res. (S)*, 1978, 254 (*struct*)

$CCl_7IrOSn_2^{2\ominus}$

IC-002377

Carbonylchlorobis(trichlorostannyl)iridate(2−), 9Cl

[61347-92-0]

$[(Cl_3Sn)_2IrCl(CO)]^{2\ominus}$

M 705.8 (ion)
Reacts with O_2, H_2 and CO.
Bis-Et_4N salt: [58146-94-4].
Ir ν_{CO} 2020 cm^{-1}.

Yurchenko, E.N. *et al*, *Koord. Khim.*, 1975, **1**, 1406 (*mössbauer, pe, ir*)
Elizarova, G.L. *et al*, *React. Kinet. Catal. Lett.*, 1975, **2**, 349 (*synth, props*)

$CCl_7OPdSn_2^{\ominus}$

IC-002378

Carbonylchlorobis(trichlorostannyl)palladate(1−), 9Cl

$[PdCl(SnCl_3)_2(CO)]^{\ominus}$

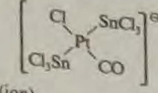
M 620.0 (ion)
Et_4N salt: [26221-09-0].
Orange solid. Anion geometry not specified.

Kingston, J.V. *et al*, *J. Chem. Soc. A*, 1971, 3765 (*synth, ir*)

$CCl_7OPtSn_2^{\ominus}$

IC-002379

Carbonylchlorobis(trichlorostannyl)platinate(1−), 11Cl



trans-form

M 708.6 (ion)
trans-form [83780-29-4]
Tetrabutylammonium salt: [103257-84-7].
$C_{17}H_{36}Cl_7NOPtSn_2$ M 951.1
Yellow-orange solid (CH_2Cl_2).

Anderson, G.K. *et al*, *Inorg. Chem.*, 1983, **22**, 427 (*synth, Sn-119 nmr, Pt-195 nmr*)
Herbert, I.R. *et al*, *Inorg. Chim. Acta*, 1986, **112**, 29 (*synth, cmr, Sn-119 nmr, Pt-195 nmr*)

$CCl_{12}OPtSn_4^{2\ominus}$

IC-002380

Carbonyltetrakis(trichlorostannyl)platinate(2−), 11Cl

$[Pt(CO)(SnCl_3)_4]^{2\ominus}$

M 1123.3 (ion)
Fluxional in soln.
Bis-Ph_4P salt: [102482-06-4].
$C_{49}H_{40}Cl_{12}OP_2PtSn_4$ M 1802.1
Orange solid (CH_2Cl_2).

Herbert, I.R. *et al*, *Inorg. Chim. Acta*, 1986, **112**, 29 (*synth, cmr, Sn-119 nmr, Pt-195 nmr*)

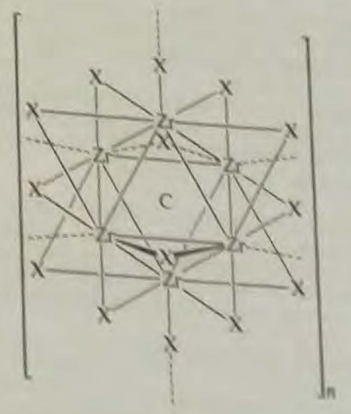
$CCl_{14}Zr_6$

IC-002381

Dodeca-μ-chlorodichloro-μ_6-methanetetraylhexazirconium, 11Cl

Zirconium carbide chloride (Zr_6CCl_{14}). *Carbidododeca-μ-chlorodichlorohexazirconium*

[96929-15-6]



X = Cl

M 1055.6
Octahedron of Zr with 12 edge-bridging Cl and C at the centre of the octahedron. Synth. by heating $ZrCl_4$, Zr and C in a sealed Ta tube to 700-860°. Reddish cryst. $Zr_6Cl_{13}C$ is also known. Be, B, N and alkali metals form similar species.

Ziebarth, R.P. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 4571 (*synth, cryst struct*)

$CCoO_3$ IC-002382

Cobalt(*III*) carbonate ($CoCO_3$)

Carbonic acid, cobalt(2+) salt (1:1)

[513-79-1]

$CoCO_3$

M 118.9

The anhyd. salt is formed from hexahydrate at 140° in a sealed tube. Commercially available. Pigment for ceramics. Light red solid consisting of microscopic rhombohedra. V. spar. sol. H_2O, EtOH, MeOAc. Dec. at 280°, weak ferromagnet.

Hexahydrate: Violet-red solid. Loses $6H_2O$ at 140°.

Mineral-form

Spharocobaltite. *Spherocobaltite. Cobaltocalcite. Cobalt spar*

Calcite-type struct. Found in Saxony, Germany assoc. with roselite, erythrite and annabergite. Rose-red to grey-brown or black translucent solid.

Remy, H., *Treatise on Inorg. Chem.*, Elsevier, 1956, **2**, 301 (*synth, props*)

Inorg. Synth., 1963, **6**, 189 (*synth*)

Moreau, R., *Bull. Soc. R. Sci. Liege*, 1967, **36**, 637 (*thermal dec*)

Rutt, H.N. *et al*, *J. Phys. C*, 1974, **7**, 4522 (*raman*)

Ehrhardt, H. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **465**, 83 (*high pressure synth*)

Le Paillier-Malecot, A., *J. Quant. Spectrosc. Radiat. Transfer.*, 1983, **29**, 231 (*uv-vis*)

Pertlik, F., *ACRC. Cryst. Struct. Commun.*, 1986, **42**, 4 (*cryst struct*)

Merck Index, 11th Ed., 1989, No. 2430.

[CCr] IC-002383

Chromium carbides

[11130-49-7]

Chromium carbide ($Cr_{23}C_6$) [12105-81-6]

C_6Cr_{23} M 1267.9

Complex fcc struct. Synth. by arc-melting Cr and C under argon. Cryst. Mp 1550° dec.

Chromium carbide (Cr_7C_3) [12075-40-0]

C_3Cr_7 M 400.0

Hexagonal struct. Isostructural with Mn_7C_3. Used in alloys and refractory coatings. Cryst. or powder. Mp 1665°. As powder, oxidises ~700°.

Chromium carbide (Cr_3C_2) [12012-35-0]

C_2Cr_3 M 180.0

Orthorhombic. The Cr atoms form trigonal prisms sharing edges with other prisms. The C atoms are found in the centres of the prisms. Obt. from pure Cr_2O_3 and carbon black heated at 1600° in presence of H_2. Used in acid- and wear-resistant alloys and refractory materials. Grey. Mp 1810°. Mp 1895°.

Chromium carbide (*CrC*) [12011-60-8]

CCr M 64.0

Various other phases known.

[12011-61-9, 12011-63-1, 12075-39-7, 12115-65-0, 12169-46-9, 12287-02-4, 12325-98-6, 12385-68-1, 12427-37-1, 12538-08-8, 12540-12-4, 12542-51-7, 12549-28-0, 12552-55-5, 74188-14-0, 77908-34-0, 92438-84-3, 96118-50-2, 110771-78-3, 112510-35-7, 123033-85-2]

Gmelin Handbook Inorg. Chem., Syst. No. 52, 1962, **B**, 352 (*rev, diffr*)

Storms, E.K., *The Refractory Carbides*, Academic Press, N. Y., 1967, 102 (*rev, diffr*)

Rundqvist, S. *et al*, *Acta Chem. Scand.*, 1969, **23**, 1191 (*synth, cryst struct: Cr_7C_3*)

Rouault, M.A. *et al*, *Ann. Chim.*, 1970, **5**, 461 (*struct: Cr_3C_2*)

Bowman, A.L. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 1502 (*cryst struct, synth: $Cr_{23}C_6$*)

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1984, **4**, 498.

CCsN

Caesium cyanide (CsCN), 8CI IC-002384

[21159-32-0]

CsCN

M 158.9

Adopts CsCl - type struct. Prepd. by addition of HCN mixed with C_2H_4 to CsOH dissolved in EtOH or similar non-aq. solv. Colourless cubic cryst. Hygroscopic. Moisture sensitive. Hydrol. to form either HCN and CsOH (< 50°) or NH_3 and $HCOOCs$ (> 80°). Transforms to a ferroelectrically ordered trigonal phase at −80°. Mp 528°. ΔH_f° −121 kJ mol^{-1}.

▷ Highly toxic.

Sugisaki, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 1567 (*synth*)

Lalild, M.F.C., *Trans. Faraday Soc.*, 1969, **65**, 2713 (*thermochem data*)

Lindl, A. *et al*, *J. Phys. C*, 1980, **13**, L349 (*luminescence, theor*)

Seaverdis do Carmo, L.C. *et al*, *Phys. Rev. B*, 1981, **23**, 5139 (*ir*)

Knoepp, G. *et al*, *Z. Phys. B*, 1983, **52**, 259 (*polymorphism*)

Eschner, S. *et al*, *Z. Phys. B*, 1983, **52**, 17 (*N-14, Cs-133 nmr*)

Stevenson, K. *et al*, *J. Chem. Phys.*, 1985, **83**, 2435 (*high press polymorphism*)

De Long, M.C. *et al*, *J. Crystal Growth*, 1986, **75**, 164 (*synth, props*)

Moodbrook, S. *et al*, *J. Magn. Reson.*, 1986, **66**, 362 (*Cs-133 nmr*)

CCs_2O_3 IC-002385

Caesium carbonate (Cs_2CO_3)

Carbonic acid, dicaesium salt, 8CI

[534-17-8]

Cs_2CO_3

M 325.8

Prepd. by reaction of aq. CsOH with CO_2 at 1250-3000 atm. and 100-110°. Commercially available. Reagent for the synth. of crown ethers and macrocyclic lactones. Dissolution in acids affords the corresp. Cs salts. Deliquescent colourless monoclinic cryst. V. sol. H_2O (261 g per 100 cm^3 at 15°); sol. EtOH (11 g per 100 cm^3 at 19°); sol. Et_2O. ΔH_f° −1119 kJ mol^{-1}. Dec. at 610° with CO_2 loss.

▷ Irritant; corrosive. FK9400000.

Gmelin Handbook Inorg. Chem., Syst. No. 25, 1955, 234 (*rev, bibl*)

Piepers, O. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 383 (*uses*)

van Keulen, B.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 281 (*uses*)

Yoshigaki, H., *Ann. Acad. Braz. Cienc.*, 1980, **52**, 521; *CA*, 1981, **94**, 75081 (*ir, raman, cryst struct*)

Ehrhardt, H. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **462**, 185 (*synth, cryst struct*)

Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 746.

$CCuF_3O_3S$ IC-002386

Trifluoromethanesulfonic acid copper(1+) salt, 9CI

Copper(I) triflate. Copper(I) trifluoromethanesulfonate

[42152-44-3]

$CuOSO_2CF_3$

M 212.6

Catalyst for olefin dimerisation, cyclopropanation and carbene addn., for promotion of Grob-type

fragmentations and in Ullmann reactions. Used to separate alkenes (e.g. ethene) from other hydrocarbons and CO. Complexes C_6H_6 and a range of polyenes. Activates C-H bonds in alkynes. Reagent for mild dehydration of alcohols. Air- and moisture-sensitive. Prepd. *in situ*.

CO adduct: [81987-72-8]

$C_7CuF_3O_5S$ M 240.6

Near white microcryst. (v. pale pink). Sol. Et_2O. Stable indefinitely under CO. Limited air stability. Forms adducts with phen., bipy, TMED. Phosphines displace CO. Ir ν_{CO} 2118 cm^{-1}.

Cyclohexene complex (1:1): Cyclohexene copper trifluoromethanesulfonate

$C_7H_{10}CuF_3O_3S$ M 294.7

Possible catalyst in photochemically induced alkene insert. White cryst. Sol. toluene.

U.S. Pat., 3 763 200, (1971); *CA*, **80**, 70278x (*use*)

Salomon, R.E. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 1889 (*derivs*)

Dines, M.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 12 (*derivs, cryst struct*)

Masamune, S. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 6756 (*use*)

Evans, J.Th.M. *et al*, *Tetrahedron Lett.*, 1978, 821, 2317, 2321 (*use*)

Salomon, R.G. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 3961 (*use*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **5**, 151-152; **6**, 130-133; **7**, 76-76; **8**, 125-126; **10**, 108-110; **11**, 142-143.

Org. Synth., 1980, **59**, 202 (*synth, use*)

Nagayoshi, K.G. *et al*, *Chem. Lett.*, 1983, 1355 (*use*)

Doyle, G. *et al*, *Inorg. Chem.*, 1983, **22**, 2893 (*derivs*)

Timmermans, P.J.J.A., *Tetrahedron Lett.*, 1983, **24**, 1419 (*use*)

Kranitli, K. *et al*, *J. Org. Chem.*, 1984, **49**, 4322 (*use*)

Hollins, J.G. *et al*, *J. Organomet. Chem.*, 1984, **260**, 369 (*use*)

Timmermans, P.J.J.A. *et al*, *J. Organomet. Chem.*, 1984, **276**, 287 (*derivs, cryst struct*)

Salomon, R.G. *et al*, *Tetrahedron Lett.*, 1984, **24**, 3167 (*use*)

Lasitli, K. *et al*, *Helv. Chim. Acta*, 1987, **70**, 607 (*use*)

Stang, P.J. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 228 (*use*)

Ghosh, S. *et al*, *J. Org. Chem.*, 1987, **52**, 83 (*use*)

CCuN IC-002387

Copper cyanide, 9CI

Cuprous cyanide. Cupricin

[544-92-3]

CuCN

M 89.5

Insecticide, fungicide. Catalyses addition of dialkyl(dimethylphenylsilyl)zinclithium to acetylenes. Reagent in prep. of acyl trimethylsilanes from carboxylic acid derivs. Catalyses allylation of zinc esters. White-cream powder, dark-green orthorhombic cryst. or dark-red monoclinic cryst. Sol. NH_3 aq., insol. H_2O, alcohols. Mp 474°.

▷ Poisonous. GL7150000.

$NHEt_2$ complex:

$C_9H_{11}CuN_2$ M 162.7

Colourless cryst. Sol. THF.

NEt_3 complex:

$C_9H_{19}CuN_2$ M 190.7

Colourless cryst. Sol. CH_2Cl_2.

Phen complex: see (*Cyano-C*)(*1,10-phenanthroline-N^1,N^{10}*) *copper, IC-008401*

4-Me-Py complex (2:3):

$C_{20}H_{21}Cu_2N_5$ M 458.5

Colourless cryst. Sol. 4-methylpyridine.

Barber, H.J., *J. Chem. Soc.*, 1943, 79 (*synth*)

Norberg, B. *et al*, *Acta Chem. Scand., Ser. A*, 1949, **3**, 174 (*synth*)

Vaughan, W.R. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 2504 (*use*)

Penneman, R.A. *et al*, *J. Chem. Phys.*, 1956, **24**, 293 (*ir*)

Cromer, D.T. *et al*, *Acta Crystallogr.*, 1965, **19**, 192.

Chadwick, B.M. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1966, **8**, 153 (*rev, synth*)

Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Interscience, New York, 1976, 266.

Denny, G. *et al*, *Cryst. Struct. Commun.*, 1982, **11**, 1805.

Stansfield, F., *J. Chem. Soc., Perkin Trans. 1*, 1984, 2933.

Terashima, M. *et al*, *Heterocycles*, 1985, **23**, 117 (*use*)

Dyason, J.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 839.

Okuda, Y. *et al*, *Tetrahedron Lett.*, 1985, **26**, 4629 (*use*)

Knochel, P. *et al*, *Tetrahedron Lett.*, 1986, **27**, 4427, 4431 (*use*)

Ochiai, H. *et al*, *J. Org. Chem.*, 1987, **52**, 4418 (*use*)

Kang, J. *et al*, *Tetrahedron Lett.*, 1987, **28**, 3261 (*use*)

CCuNS

Copper(*I*) thiocyanate IC-002388

Cuprous thiocyanate

[1111-67-7]

CuSCN

M 121.6

Precipitates from $CuSO_4$-NH_4NCS-$NaHSO_3$-H_2O systems. Used in marine anti-fouling paints. White cryst. (α-form) or brown cryst. (β-form). Prac. insol. H_2O, EtOH, Me_2CO. Mp 1084°.

Demmerle, R.L. *et al*, *Ind. Eng. Chem.*, 1950, **42**, 2 (*synth*)

Kabesova, M. *et al*, *Inorg. Chim. Acta*, 1976, **17**, 161; 1978, **31**, L435 (*synth, cryst struct, ir*)

Smith, D.L. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 907 (*cryst struct*)

Merck Index, 11th Ed., 1989, No. 2676.

$CCuO_3$ IC-002389

Copper(*II*) carbonate ($CuCO_3$)

Cupric carbonate. Carbonic acid copper(2+) salt (1:1), 9CI

[1184-64-1]

$CuCO_3$

M 123.5

Struct. comprises coplanar CuO_4 chains linked into stacked sheets by bidentate $(CO_3)^{2\ominus}$. Fungicide. Catalyst. Cryst.

[7492-68-4, 36386-77-3]

Graf, D.L., *Am. Mineral.*, 1961, **46**, 1283 (*cryst struct*)

Seidel, V.H. *et al*, *Z. Anorg. Allg. Chem.*, 1974, **410**, 138 (*cryst struct*)

[CDy] IC-002390

Dysprosium carbides

Known phases include Dy_3C, Dy_2C_3, DyC_2.

Dysprosium carbide (*DyC_2*) [12175-80-3]

C_2Dy M 186.5

Possesses CaC_2 struct. Yellow powder. On hydrolysis affords mainly C_2H_2 but also C_2H_4, C_2H_6 and other hydrocarbons. $\alpha \rightarrow \beta$ transition at 1295° (1250°). Undergoes antiferromagnetic of ordering at 61K. μ_{eff} = 10.53μ_B (θ −68.9°).

[56780-66-6]

Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*struct*)

Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, magnetism*)

Adachi, G. *et al*, *J. Less-Common Met.*, 1973, **32**, 301 (*struct*)

Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)

Male, G., *Rev. Int. Hautes Temp. Refract.*, 1977, **14**, 179 (*synth*)

Sakai, T. *et al*, *Mater. Res. Bull.*, 1980, **15**, 1001 (*magnetism*)

Barak, Z. *et al, Phys. Rev. B*, 1982, **25**, 1965 (*magnetism*)
Karen, P. *et al, Collect. Czech. Chem. Commun.*, 1986, **51**, 1411 (*hydrol*)

IC-002391

[CEr]

Erbium carbides

Phases known include Er_3C, ErC_2.

Erbium carbide ***(ErC_2)*** [12192-37-9]

C_2Er M 191.2

Possesses CaC_2 struct. Yellow solid. Antiferromagnetic below 19K. On hydrol. affords mainly C_2H_2 but with some C_2H_4, C_2H_6 and other hydrocarbons. Undergoes $\alpha \rightarrow \beta$ transition at 1325° (1275°). $\mu_{eff} = 8.75\mu_B$ (θ 14.7°).

Spedding, F.H. *et al, J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al, J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, magnetism*)
Atoji, M. *et al, J. Chem. Phys.*, 1972, **57**, 2410 (*nd, cryst struct*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Sakai, T. *et al, J. Less-Common Met.*, 1981, **81**, 91 (*magnetism, conductivity*)

[CEu] IC-002392

Europium carbides

Known phases include Eu_3C, Eu_2C_3, EuC_2.

Europium carbide ***(EuC_2)*** [12127-44-5]

C_2Eu M 175.9

Studied as possible neutron absorber in nuclear reactors. Black powder. Dec. by H_2O. Undergoes phase transition at 350°. Ferromagnetic, $T_c \sim 20K$.

Gebelt, R.E. *et al, Inorg. Chem.*, 1964, **3**, 335 (*synth, struct*)
Colquhoun, I. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1337 (*synth, mössbauer*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Schwetz, K.A. *et al, Ceram. Int.*, 1979, **5**, 105; *CA*, **93**, 56143 (*use*)
Sakai, T. *et al, Bull. Chem. Soc. Jpn.*, 1982, **55**, 609 (*synth, magnetism*)

$CEuO_3$ IC-002393

Europium(*II*) carbonate ($EuCO_3$)

[5772-74-7]

$EuCO_3$

M 211.9

Isostructural with KNO_3. Useful source of $Eu^{2\oplus}$ salts on reaction with acid. Lemon-yellow solid. Insol. H_2O. Dec. to $Eu_2O(CO_3)_2$ at 430°, and to Eu_2O_3 at 660°.

Inorg. Synth., 1946, **2**, 71 (*synth*)
Sklyarenko, Yu.S. *et al, CA*, 1973, **79**, 60958 (*synth, thermal dec, struct*)
Sterzel, W. *et al, Z. Anorg. Allg. Chem.*, 1976, **392**, 173 (*ir*)

CFIO IC-002394

Carbonic fluoride iodide, 9CI

Carbonyl fluoride iodide, 8CI. Fluoroiodophosgene

O=CFI

M 173.9

Synth. from IF_5 + CO. Colourless gas, slowly hydrol. by H_2O. Mp −120°. Bp −20.6°. Dec. above −20°.

▷ Presumed toxic.

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 225 (*synth*)

CFN IC-002395

Cyanogen fluoride, 9CI, 8CI

Fluorine cyanide. Fluoroformonitrile

[1495-50-7]

FC≡N ($C_{\infty v}$)

M 45.0

Interatomic distances: F—C 126, C—N 116.5 pm. Synth. by pyrolysis of $(CNF)_3$. Colourless gas, stable at −78°. Mp −82°. Subl. −72°, Bp −46°.

▷ Can polymerise expolsively.

Fawcett, F.S. *et al, J. Am. Chem. Soc.*, 1960, **82**, 1509 (*synth, props*)
Taylor, J.K. *et al, Trans. Faraday Soc.*, 1963, **59**, 2661 (*struct*)
Kemmitt, R.D.W. *et al, Adv. Fluorine Chem.*, 1965, **4**, 142 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 227 (*synth*)
Bieri, G., *Chem. Phys. Lett.*, 1977, **46**, 107 (*uv*)
Shimanouchi, T., *J. Phys. Chem. Ref. Data*, 1977, **6**, 993 (*ir*)
Bauknight, C.W. *et al, J. Org. Chem.*, 1988, **53**, 4443 (*synth, haz*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 988.

CFN IC-002396

Isocyanogen fluoride

Fluoroisocyanide

[16992-26-0]

FN≡C

M 45.0

Identified spectroscopically by photolysis of matrix-isolated FCN.

Milligan, D.E. *et al, J. Chem. Phys.*, 1967, **47**, 278 (*spectra*)

CFNO IC-002397

Fluorine isocyanate

Fluoroisocyanate

[42088-15-3]

FN=C=O

M 61.0

Formed in Ar matrix by photolysis of $FCON_3$ or $XCONF_2$ compds. (X = H, NH_2, CF_3).

Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 137 (*bibl*)
Khodayar, G. *et al, Z. Naturforsch., B*, 1984, **39**, 1211 (*matrix isol*)

$CFNO_3S$ IC-002398

Fluorosulfuryl isocyanate

Sulfuryl fluoride isocyanate

[1495-51-8]

$FSO_2N=C=O$

M 125.0

Best synth. from $ClSO_2NCO$ + phenyl carbamoyl fluoride. Colourless liq. Bp 61.5°.

Appel, R. *et al, Chem. Ber.*, 1964, **97**, 849; 1975, **108**, 582; 1976, **109**, 2437 (*synth, ms, reactions, F-19 nmr*)
Noftle, R.E. *et al, Inorg. Chem.*, 1968, **7**, 687 (*synth, ir, F-19 nmr, reactions*)

CFN_3O IC-002399

Carbonazidic fluoride

[23143-88-6]

$(N_3)C(O)F$

M 89.0

Synth. from COClF + NaN_3 at 25°. Colourless liq. Bp 36°.

Gholivand, K. *et al, Z. Naturforsch., B*, 1984, **39**, 1211 (*synth, ir, raman, ms, F-19 nmr, props*)

IC-002400

CF_2I_2

Difluorodiiodomethane, 9CI

[1184-76-5]

CF_2I_2

M 303.8

Yellow liq. Mp −72°. Bp 80.5° (calc.).

Mahler, W., *Inorg. Chem.*, 1963, **2**, 230 (*synth, ir, uv*)
Mitsch, R.A., *J. Heterocycl. Chem.*, 1964, **1**, 233 (*synth, nmr, uv, ir*)
McAlpine, I. *et al, Spectrochim. Acta, Part A*, 1969, **25**, 1723 (*ir*)
Elsheimer, S. *et al, J. Org. Chem.*, 1984, **49**, 205 (*synth, fmr, cmr, ir, props*)

CF_2NOP IC-002401

Difluoroisocyanatophosphine, 8CI

Phosphorisocyanatidous difluoride, 9CI, 8CI. Difluoro(cyanato-N)phosphorus(III)

[461-59-6]

O=C=NPF_2

M 110.9

Interatomic distances (vap.): P—F 156.3, P—N 168.3, N—C 125.6, C—O 116.8 pm; angle: PNC 130.6°. Synth. from Phosphorous triisocyanate, IC-003783 + SbF_3. Low boiling liq. of poor stability. V. reactive to protic compds. Spar. sol. CS_2. d_4^{20} 1.444. Mp −108°. Bp 12.3°. n_D^{20} 1.3695.

Anderson, H.H., *J. Am. Chem. Soc.*, 1947, **69**, 2495 (*synth*)
Fluck, E., *Z. Naturforsch., B*, 1964, **19**, 869 (*P-31 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 628 (*rev, bibl*)
Flaskerud, G.G. *et al, Inorg. Chem.*, 1969, **8**, 728 (*ir, ms, F-19 nmr*)
Rankin, D.W.H. *et al, Inorg. Nucl. Chem. Lett.*, 1972, **8**, 1101 (*ms*)
Rankin, D.W.H. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1277 (*ir, raman, ed*)
Cradock, S. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 940 (*pe*)

CF_2NOPS IC-002402

Isocyanatodifluorophosphine sulfide

Phosphorisocyanatidothioic difluoride, 9CI, 8CI. Difluoroisocyanatothioxophosphorus(V)

[27961-68-8]

O=C=NP(S)F_2

M 143.0

Synth. from PSF_3 + $Si(NCO)_4$. Colourless, odourless liq. Moisture sensitive. d_4^{20} 1,430. Bp 46-47°. n_D^{20} 1.3920.

▷ Inflames in air.

Colburn, C.B. *et al, J. Chem. Soc. A*, 1970, 2221 (*synth, ir, ms, F-19 nmr*)
Roesky, H.W., *J. Inorg. Nucl. Chem.*, 1970, **32**, 1845 (*synth, ir, ms, F-19 nmr*)
Shokol, V.A. *et al, Zh. Obshch. Khim.*, 1971, **41**, 1406; *J. Gen. Chem. USSR (Engl. Transl.)*, 1971, **41**, 1412 (*synth*)

CF_2NP IC-002403

Phosphorocyanidous difluoride, 9CI

Cyanodifluorophosphine. Cyanodifluorophosphorus(III)

[14118-40-2]

F_2PCN

M 94.9

Colourless volatile liq., quite unstable even at −20°.

Rudolph, R.W. *et al, J. Am. Chem. Soc.*, 1966, **88**, 3729 (*synth, ir, raman, F-19 nmr, P-31 nmr*)
Holywell, G.C. *et al, J. Mol. Struct.*, 1971, **9**, 11 (*ed*)
Lee, P.L. *et al, Inorg. Chem.*, 1972, **11**, 1917 (*microwave, nqr, struct*)
Cradock, S. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 940 (*pe*)
Harland, P.W. *et al, Inorg. Chem.*, 1973, **12**, 1442 (*synth, ms*)
Hall, W.R. *et al, Inorg. Chem.*, 1973, **12**, 1878 (*struct*)
Leibovici, C., *J. Mol. Struct.*, 1973, **18**, 343 (*struct*)
Howell, J.M. *et al, Chem. Phys. Lett.*, 1976, **39**, 312 (*struct*)
Cox, A.W. *et al, Inorg. Chem.*, 1977, **16**, 2048 (*ir, raman*)

CF_2N_2 IC-002404

Difluorocyanamide

[7127-18-6]

$F_2NC≡N$

M 78.0

Interatomic distances: C≡N 115.8, C—N 138.6, N—F 139.9 pm, angle: NCN 174°. Formed from H_2NCN + F_2/He. Colourless gas.

▷ Highly explosive.

Meyers, M.D. *et al, Inorg. Chem.*, 1966, **5**, 1455 (*synth, F-19 nmr*)
Lee, P.L. *et al, Inorg. Chem.*, 1972, **11**, 1920 (*microwave*)

CF_2O IC-002405

Carbonyl fluoride

Carbonic difluoride, 9CI. Fluophosgene

[353-50-4]

COF_2 (C_{2v})

M 66.0

Synth. from CO and AgF_2 or from CO and F_2. Hygroscopic, colourless gas. Highly reactive C—F bonds. Readily hydrol. to CO_2 and HF. d^{-114} 1.139. Mp −114.0°. Bp −83.1°.

▷ Highly toxic by inhalation, irritant, TLV 15. FG6125000.

Inorg. Synth., 1960, **6**, 155 (*synth*)
Fawcett, F.S. *et al, J. Am. Chem. Soc.*, 1962, **84**, 4275 (*synth*)
Sheppard, W.A. *et al, J. Org. Chem.*, 1964, **29**, 1, 11 (*use*)
Kemmitt, R.D.W. *et al, Adv. Fluorine Chem.*, 1965, **4**, 142 (*rev*)
Fieser, M. *et al, Fieser and Fieser, Reagents for Organic Synthesis*, Wiley, 1967-1984, **1**, 116 (*use*)
Carpenter, J.H., *J. Mol. Spectrosc.*, 1974, **50**, 182 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 223 (*synth*)
Gupta, O.D. *et al, J. Chem. Soc., Chem. Commun.*, 1984, 416 (*use*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 717.

IC-002406

$CF_2O_3Pb_2$

Lead carbonate fluoride ($Pb_2(CO_3)F_2$)

Dilead difluoride carbonate. [μ-[Carbonato(2−)-O:O′]] difluorodilead, 11CI

[86508-50-1]

$Pb_2F_2(CO_3)$

M 512.4

Struct. comprises endless spiral chains of edge-sharing FPb_4 tetrahedra joined by corner sharing to a 3-D network of $(PbF)_n^{n\oplus}$. The $CO_3^{2\ominus}$ are situated in the tunnels of this network. Orthorhombic cryst.

Aurivillius, B., *Acta Chem. Scand., Ser. A*, 1983, **37**, 159.

IC-002407

CF_2S

Thiocarbonyl fluoride

Carbonothioic difluoride, 11Cl, 9Cl

[420-32-6]

$S{=}CF_2$ (C_{2v})

M 82.0

Interatomic distances: F—C 131.5, C—S 158.9 pm; bond angle: FCF 107.1°. Synth. from Cl_2CS + KF. Gas. Mp −163.5°. Bp −62.6°, Bp −62.1°, Bp −54°. Polymeric form also known.

S-oxide. [63674-05-5]. *Difluoromethylene sulfoxide*

CF_2OS M 98.0

Synth. from $(F_2CS)_2$ + CF_3CO_3H. Dec. at −100° to F_2CO + S.

[25610-08-6]

Downs, A.J., *J. Chem. Soc.*, 1962, 4361 (*synth, ir, nmr, uv*)
Kennitt, R.D.W. *et al*, *Adv. Fluorine Chem.*, 1965, **4**, 142 (*rev*)
Middleton, W.J. *et al*, *J. Org. Chem.*, 1965, **30**, 1375 (*synth, nmr*)
Careless, A.J. *et al*, *Chem. Phys.*, 1973, **1**, 371 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 641 (*synth*)

CF_2Se

IC-002408

Selenocarbonyl difluoride

Carbonoselenoic difluoride, 11Cl, 9Cl. Difluoroselenoformaldehyde. Selenoyl fluoride

[54093-39-4]

$Se{=}CF_2$

M 128.9

Polymerises in the presence of Lewis acids.

Dimer: see *2,2,4,4-Tetrafluoro-1,3-diselenetane, IC-002929*

Haas, A. *et al*, *Chem.-Ztg.*, 1974, **98**, 511; *CA*, **82**, 97622 (*synth*)
Haas, A. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 487 (*raman, ir*)
Gombler, W., *Z. Naturforsch., B*, 1981, **36**, 1561 (*Se-77 nmr, cmr*)

CF_3IS

IC-002409

Trifluoromethanesulfenyl iodide, 9Cl

[102127-62-6]

F_3CSI

M 227.9

Orange-yellow solid at −108°.

Minkwitz, R. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **527**, 161 (*synth, F nmr, cmr, ir, raman*)

CF_3LiO_3S

IC-002410

Lithium trifluoromethanesulfinate

Trifluoromethanesulfinic acid, lithium salt, 8Cl. Lithium triflite

[33454-82-9]

$LiOS(O)CF_3$

M 156.0

When mixed with poly(ethylene oxide) forms thin polymer electrolyte films which exhibit high ionic conductivity. Commercially available. Electrolyte component for lithium batteries.

▷ Irritant.

Bennion, D.N. *et al*, *J. Chem. Eng. Data*, 1971, **16**, 368 (*phys props*)
Watanabe, M. *et al*, *Kinzoku Hyomen Gijutsu*, 1986, **37**, 214; *CA*, 1986, **105**, 104503 (*uses*)
Ito, Y. *et al*, *Solid State Ionics*, 1986, **18-19**, 277 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2159D (*haz*)

CF_3N

Fluorocarbonimidic difluoride

IC-002411

Fluoroiminodicarbonyl fluoride, 8Cl. Trifluoromethylenimine. Perfluoromethylenimine

[338-66-9]

$F_2C{=}NF$

M 83.0

Gas with odour resembling HCN. Bp −60°.

▷ Explodes on strong heating.

Dybvig, D.H., *Inorg. Chem.*, 1966, **5**, 1795 (*nmr, ir, ms*)
Ginsburg, V.A. *et al*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, 1343 (*synth, ir, ms*)

CF_3NO

Difluorocarbamic fluoride, 9Cl

IC-002412

Difluorocarbamoyl fluoride, 8Cl. Difluoraminocarbonyl fluoride

[2368-32-3]

F_2NCOF

M 99.0

Synth. from N_2F_4 + CO + hν. Gas. Colourless glass below −130°. d 1.63 at −78°. Mp −152.2°. Bp −32° (extrap.), −82.4°. Hydrol. immediately by H_2O. Vp 160 mm at −78°. Reduced by HI.

▷ Highly toxic, strong oxid. agent requiring special apparatus for handling.

Ruff, O. *et al*, *Ber.*, 1936, **69**, 598, 684 (*synth*)
Fraser, G.W. *et al*, *Inorg. Chem.*, 1965, **4**, 1497 (*synth, ms, ir, nmr*)
Inorg. Synth., 1970, **12**, 299 (*synth, use, ir*)

CF_3NO

IC-002413

Trifluoronitrosomethane, 8Cl

[334-99-6]

F_3CNO

M 99.0

Industrial intermed. in synth. of nitroso rubbers. Deep-blue gas condensing to a deep-blue liq. and freezing to a purple solid. Mp −196.6°. Bp −84°.

Dimer:

$C_2F_6N_2O_2$ M 198.0

Formed reversibly on uv or vis irradiation. Orange-red. Has struct. $(F_3C)_2N{-}ONO$ (distinction from other nitroso compds.).

Haszeldine, R.N., *J. Chem. Soc.*, 1953, 2075 (*synth*)
Dubov, S.S. *et al*, *Zh. Obshch. Khim.*, 1964, **34**, 1961; *CA*, **61**, 7026c (*rev*)
Dinwoodie, A.R. *et al*, *J. Chem. Soc.*, 1965, 1675 (*synth*)
Mason, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1969, 257 (*nmr*)
Umemoto, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 820 (*synth*)

CF_3NOS

IC-002414

(Fluorocarbonyl)imidosulfurous difluoride, 9Cl

(Fluoroformyl)imidosulfurous difluoride, 8Cl. N-(Fluoroformyl)iminosulfur difluoride. S,S-Difluoro-N-(fluoroformyl)sulfilimine

[3855-41-2]

$F_2S{=}NCOF$

M 131.0

Primary starting material in S—N—F chemistry. Colourless pungent liq. Mp −95°. Bp 48.8° (54°). Dec. at 190° to COF_2 and NSF, or at 0° in presence of $F^\ominus$.

▷ Highly toxic.

Clifford, A.F. *et al*, *Inorg. Chem.*, 1965, **4**, 571 (*synth, ms, uv, ir, nmr*)
Biermann, U. *et al*, *Chem. Ber.*, 1967, **100**, 3795 (*synth, ms, ir, nmr*)
Inorg. Synth., 1986, **24**, 10 (*synth, ir, F-19 nmr*)

CF_3NO_4

IC-002415

Trifluoromethyl peroxynitrate

Peroxynitric acid, trifluoromethyl ester, 9Cl

[50311-48-3]

F_3COONO_2

M 147.0

Colourless gas. Bp 0.9° (extrap.). Dec. at 127° to COF_2 + NO_2 + O_2.

▷ Explosive.

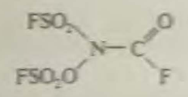
Hohorst, F.A. *et al*, *Inorg. Chem.*, 1974, **13**, 715 (*synth, ir, raman, ms, props*)

$CF_3NO_4S_2$

IC-002416

N-(Fluoroformyl)-*N*,*O*-bis(fluorosulfonyl)hydroxylamine, 8Cl

[19252-48-3]



M 243.1

Synth. from FSO_2NCO + $FOSO_2F$ + hν. Colourless liq., hydrol. in moist air. Bp 121.8°.

Noble, R.E. *et al*, *Inorg. Chem.*, 1968, **7**, 687 (*synth, ir, F-19 nmr, props*)

CF_4

IC-002417

Carbon tetrafluoride

Tetrafluoromethane, 9Cl. Perfluoromethane. Fluorocarbon 14

[75-73-0]

CF_4

M 88.0

Low temp. refrigerant, gaseous insulator. Gas. Spar. sol. H_2O. Mp −183.6°. Bp −128°.

▷ Narcotic in high concs. Reacts violently with Al. Dec. to toxic COF_2 if strongly heated in air. FG4920000

Lebeau, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1926, **182**, 1340
Simons, J.H. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 3477 (*synth*)

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 284.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 716.

CF_4N_2O

Tetrafluorourea

IC-002418

[10256-92-5]

$(F_2N)_2C{=}O$

M 132.0

Formed from $F_2NC(O)Cl$ + HgO. Colourless gas. Bp −20°.

▷ Dec. ~80°.

Wright, K.J. *et al*, *Inorg. Chem.*, 1973, **12**, 77 (*synth, ms*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, D3, 125 (*bibl*)

CF_4O

Trifluoromethyl hypofluorite

IC-002419

Fluoroxytrifluoromethane. Hypofluorous acid trifluoromethyl ester

[373-91-1]

F_3COF

M 104.0

Synth. from CO + F_2. Fluorinating and oxidising agent with synth. applications. Strong oxidising agent. Gas having odour similar to F_2 or OF_2. When liquefied has pale straw colour. Mp < −215°. Bp −95°. Stable to 450°. Hydrol. by aq. NaOH, slowly in H_2O. Above 370° dec. to COF_2 + F_2.

▷ Highly poisonous.

Kellog, K.B. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 3986 (*synth*)
Holtzmann, R.T. *et al*, *Inorg. Chem.*, 1962, **1**, 972 (*synth*)
Maraniz, L.B., *J. Org. Chem.*, 1965, **30**, 4300 (*ir, uses*)
Inorg. Synth., 1966, **8**, 165 (*synth*)
Wilt, P.M. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 2108 (*ir*)
Kennedy, R.C. *et al*, *J. Fluorine Chem.*, 1973, **3**, 41 (*synth*)
DeMarcus, R.A. *et al*, *J. Magn. Reson.*, 1975, **18**, 522 (*nmr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 653 (*synth*)
Olsen, J.F., *J. Fluorine Chem.*, 1977, **9**, 471 (*struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 156 (*use*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1261 (*haz, toxicity*)

CF_4O_2

IC-002420

Hypofluorous acid difluoromethylene ester, 11Cl, 9Cl

Difluoromethanediol dihypofluorite. Bis(fluoroxy) difluoromethane. Difluorodifluoroxymethane

[14230-67-4]

$F_2C(OF)_2$

M 120.0

Formed from CO_2 + F_2 at −78° in presence of CsF; may be prepared in glass or metal containers. Reacts with glass at elevated temps. Electrophilic fluorinating agent. Gas or pale yellow liq. Colourless liq. at −184° to −183°, glassy material (v. viscous) at −196°. d_4^{-42} 1.20. Mp < −184° (glass or syrup at −196°). Bp −62°, Bp −63°. Readily reacts with Hg. Stable at r.t. in glass or perfluorinated metal vessels.

▷ Strong oxidising agent. Potentially haz. with org. or easily oxid. materials.

Hohorst, F.A. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 1809, 3511 (*synth, ir, F-19 nmr*)

Thompson, P.G., *J. Am. Chem. Soc.*, 1967, **89**, 1811 (*synth, haz, F-19 nmr, ir*)
Cauble, R.L. *et al, J. Am. Chem. Soc.*, 1967, **89**, 1962, 5161 (*synth, ir, F-19 nmr*)
Mitchell, R.W. *et al, J. Mol. Spectrosc.*, 1967, **24**, 128 (*ir*)
Inorg. Synth., 1968, **11**, 143 (*synth, F-19 nmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 36.
Huston, J.L. *et al, J. Fluorine Chem.*, 1979, **13**, 235 (*ms*)
Walker, N. *et al, J. Magn. Reson.*, 1979, **34**, 295 (*cmr*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1254 (*haz, tox*)

IC-002421

CF_4S

Trifluoromethanesulfenyl fluoride, 9CI

[17742-04-0]

F_3CSF

M 120.0
Highly reactive substance. Forms dimer at low temp.
Stored at ambient temp. <100 mm Hg.

▷ Highly toxic.

Dimer: [26391-89-9]. *Difluoro(trifluoromethanethiolato)(trifluoromethyl)sulfur, 9CI, 8CI*
$C_2F_8S_2$ M 240.1
Dimer in equilibrium with CF_3SF. Has struct.
$F_3CSF_2-S-CF_3$.

Stump, E.C., *Chem. Eng. News*, 1967, **45**, 16 (*tox*)
Seel, F. *et al, Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 773 (*dimer, synth, fmr, props*)
Gombler, W. *et al, J. Fluorine Chem.*, 1974, **4**, 333 (*dimer, F nmr*)
Gombler, W. *et al, Z. Anorg. Allg. Chem.*, 1978, **439**, 193; 1980, **469**, 139 (*synth, ir, F nmr, ms, dimer*)
Oberhammer, H. *et al, J. Mol. Struct.*, 1981, **70**, 273 (*ed, ir, raman, bibl*)

IC-002422

CF_5NORe

(Cyanato-*N*)pentafluororhenium(*VI*), 12CI
Rhenium(VI) *pentafluoride isocyanate*

[107605-59-4]

$ReF_5(NCO)$

M 323.2
Synth. from ReF_6 and $Me_3Si(NCO)$. Air-sensitive brownish-purple solid. Dec. at 200-300°.

Fawcett, J. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 567 (*synth, ir, props*)

IC-002423

CF_4NOS

(Cyanato-*N*)pentafluorosulfur
Pentafluoro(isocyanato)sulfur

[2375-30-6]

$O{=}C{=}NSF_4$

M 169.0
From $NSF_3 + COF_2 + HF$ or from $F_5SNHCO_2Ph + PCl_5$. Colourless liq. Bp 5-5.5°.

Tullock, C.W. *et al, J. Am. Chem. Soc.*, 1964, **86**, 357 (*synth*)
Thrasher, J.S. *et al, Inorg. Chem.*, 1982, **21**, 1616 (*reactions*)
Thrasher, J.S. *et al, J. Fluorine Chem.*, 1983, **23**, 593 (*synth*)
Oberhammer, H. *et al, J. Mol. Struct.*, 1983, **101**, 325 (*ed*)
Seppelt, K. *et al, Inorg. Chem.*, 1985, **24**, 1227 (*ed, N-14 nmr, F-19 nmr, S-33 nmr*)

IC-002424

CF_5NOS

(Cyanato-*O*)pentafluorosulfur
Pentafluorosulfur cyanate

$N{\equiv}C{-}O{-}SF_5$

M 169.0
Interatomic distances: C—N 116.2; O—C 127.1, S—F 155.4, S—O 165.3 pm. Angles SOC 120.4°, OCN 175.3°
Formed from *cis*-$F_5SOCCl{=}NCl$ + Hg. Colourless gas. Mp −60°. Bp 5°.

Schmuck, A. *et al, Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 134 (*synth, F-19 nmr, N-14 nmr, ir, raman, ms*)
Zylka, P. *et al, Inorg. Chem.*, 1991, **30**, 59 (*ed*)

IC-002425

CF_5NOSe

(Cyanato-*O*)pentafluoroselenium
Pentafluoroselenium cyanate

[94994-37-3]

$N{\equiv}C{-}O{-}SeF_5$

M 215.9
Until recently thought to be $OCNSeF_5$. From $Xe(OSeF_5)_2$ + HCN. Colourless liq. Mp −79°. Bp 39°.

▷ Explosive.

Oberhammer, H. *et al, J. Mol. Struct.*, 1983, **101**, 325 (*ed*)
Huppmann, P. *et al, Inorg. Chem.*, 1984, **23**, 2217 (*synth, ir, ms*)
Damerius, R. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2821 (*Se-77 nmr*)
Seppelt, K. *et al, Inorg. Chem.*, 1985, **24**, 1227 (*synth, Se-77 nmr, F-19 nmr, N-14 nmr, ed*)

IC-002426

CF_5NOTe

(Cyanato-*N*)pentafluorotellurium(*VI*)

[86024-46-6]

$O{=}C{=}NTeF_5$

M 264.6
Synth. from $Me_3SiNHTeF_5 + COF_2$ or from $Xe(OTeF_5)_2$ + HCN. Colourless liq., readily hydrol. Mp −95°. Bp 39°.

Hart, H. *et al, Inorg. Chem.*, 1983, **22**, 2183 (*synth, ir, F-19 nmr*)
Seppelt, K. *et al, Inorg. Chem.*, 1985, **24**, 1227 (*synth, Te-125 nmr, N-15 nmr*)

IC-002427

CF_5NS

(Cyano-*N*)pentafluorosulfur
Pentafluoro(isocyano)sulfur. Sulfur-pentafluoride isocyanide

F_5SNC

M 153.0
Synth. from $F_5SN{=}CBr_2$ and Mg. Colourless gas, isom. to F_5SCN at r.t.

Thrasher, J.S. *et al, Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 1258 (*synth, ir, ms, F-19 nmr*)

IC-002428

CF_5NS

(Cyano-*C*)pentafluorosulfur, 12CI
Sulfur cyanide pentafluoride

[1512-13-6]

F_5SCN

M 153.0

Synth. from $(SCN)_2$ and dil. F_2 at −20°. Colourless stable gas. Bp −25°.

Lösking, O. *et al, Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 1255 (*synth, sp, ir, F-19 nmr*)

IC-002429

CF_5NS

(Trifluoromethyl)imidosulfurous difluoride
Trifluoromethyliminosulfur difluoride

[1512-14-7]

$F_3CN{=}SF_2$

M 153.0
Synth. from SF_4 and BrCN or NaSCN. Gaseous dielectric insulator for electrical devices. Highly reactive colourless gas, dec. by H_2O or EtOH; thermally stable. Bp −6°.

Smith, W.C. *et al, J. Am. Chem. Soc.*, 1960, **82**, 551 (*synth, ms, ir, nmr*)
Griffiths, J.E. *et al, Spectrochim. Acta, Part A*, 1969, **25**, 1355 (*ir*)
U.S. Pat., 3 674 696, (1972); *CA*, **77**, 94567 (*use*)
Walter, N. *et al, J. Magn. Reson.*, 1979, **34**, 295 (*cmr*)

IC-002430

CF_5N_3

Pentafluoroguanidine, 9CI
Perfluoroguanidine

[10051-06-6]

$(F_2N)_2C{=}NF$

M 149.0
Gas condensing to colourless liq. d_4^0 1.5. Bp −1.1°. V. reactive. Reacts readily with Hg, hydrol. rapidly even at r.t. Dec. at 205°.

▷ V. explosive in all states. Explosions initiated by shock, spark or phase transitions.

Davis, R.A. *et al, J. Org. Chem.*, 1967, **32**, 1662 (*synth, props, ms, F-19 nmr*)
Koshar, R.J. *et al, J. Org. Chem.*, 1967, **32**, 3859 (*synth*)
Firth, W.C. *et al, J. Org. Chem.*, 1973, **38**, 1083 (*reactions*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2130 (*haz*)

IC-002431

CF_6OS

Pentafluoro(fluorocarbonyl)sulfur
Pentafluorosulfur carbonyl fluoride
Pentafluoro(fluoroformyl)sulfur, 8CI

[19421-19-3]

$F_5SC(O)F$

M 174.0
Formed from $FC(O)C(O)F + S_2F_{10}$ + hv. Colourless gas, readily hydrol. Bp −10°.

Czerepinski, R. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3954 (*synth, ir, F-19 nmr*)

IC-002432

CF_6O_2S

Pentafluoro(fluoroformato)sulfur, 8CI
Pentafluorosulfur fluoroformate

[16829-25-7]

$F_5SOC(O)F$

M 190.0
Formed from $FC(O)C(O)F + F_5SOF$ + hv. Colourless liq. or gas, stable to glass, slowly hydrol. Mp ~ −78°. Bp ~5°.

Czerepinski, R. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3954 (*synth, ir, F-19 nmr*)

IC-002433

CF_6O_2S

Pentafluorosulfur peroxofluoroformate
Pentafluoro(fluoroperoxyformato)sulfur, 8CI
(Carbonofluoridoperoxoato-O)pentafluorosulfur, 10CI, 9CI

[19421-21-7]

$F_5SOOC(O)F$

M 206.0
Synth. from $F(O)COOC(O)F + F_9SOOSF_5$ + hv. Highly reactive colourless liq. Bp 25°.

Czerepinski, R. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3954 (*synth, ir, F-19 nmr*)
Des Marteau, D.D., *J. Am. Chem. Soc.*, 1972, **94**, 8933 (*hydrol*)

IC-002434

CF_6S

Trifluoro(trifluoromethyl)sulfur
Trifluoromethylsulfur trifluoride

[374-10-7]

F_3CSF_3

M 158.0
Synth. from CS_2 or $CF_3SSCF_3 + AgF_2$ at −50°. Colourless gas. Bp −7°.

Sheppard, W.A., *J. Am. Chem. Soc.*, 1962, **84**, 3058 (*synth, reactions*)
Lawless, E.W. *et al, Inorg. Chem.*, 1968, **7**, 391 (*synth, F-19 nmr, ir*)
Minkwitz, R. *et al, J. Fluorine Chem.*, 1987, **37**, 397 (*reactions*)

IC-002435

CF_8N_4

Octafluoromethanetetramine, 9CI
Tetrakis(difluoroamino)methane

[17125-65-4]

$C(NF_2)_4$

M 220.0
Synth. from $(F_2N)_2C(NFH)(NCO)$ and F_2/NaF. Colourless liq. d_4^{27} 1.68. Fp −13.5° to −12.5°. Bp 40°. Strong oxidising agent.

▷ Explosive.

Wright, C.D. *et al, J. Org. Chem.*, 1973, **38**, 1075 (*synth*)
Firth, W.C. *et al, J. Org. Chem.*, 1973, **38**, 1083, 1088 (*synth, ir, ms, props, F-19 nmr*)

IC-002436

CF_8O_2S

Pentafluoro(trifluoromethyldioxy)sulfur
Pentafluorosulfur trifluoromethyl peroxide

$F_5C{-}O{-}O{-}SF_5$

M 228.0
Synth. from $(F_5S)_2O_2 + (F_3C)_2O_2$. Colourless gas. Mp −136°. Bp 7.7°.

Merrill, C.I. *et al, J. Am. Chem. Soc.*, 1963, **85**, 909 (*synth, sp, ir*)

IC-002437

CF_8S

Pentafluoro(trifluoromethyl)sulfur, 9CI, 8CI
(Trifluoromethyl)sulfur pentafluoride

[373-80-8]

F_5CSF_3

M 196.0
Synth. electrochemically from HF + Me_2S or CS_2. Electrical insulator. Gas. Mp −86.9°. Bp −20.4°. Stable to alkali.

Silvey, G.A. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3624 (*synth*)
Clifford, A.F. *et al*, *J. Chem. Soc.*, 1953, 2372 (*synth*)
Murrill, C.L. *et al*, *Inorg. Chem.*, 1962, **1**, 215 (*F-19 nmr*)
Griffiths, J.E., *Spectrochim. Acta, Part A*, 1967, **23**, 2145 (*ir, raman*)
Marsden, C.J. *et al*, *J. Mol. Struct.*, 1985, **131**, 299 (*struct, rel*)

IC-002438

CF_4S_2

Pentafluorothiomethyldynesulfur(*VI*) trifluoride

Octafluoro-μ-methanetetrayldisulfur, 12Cl

[117146-26-6]

$F_5SC{\equiv}SF_3$

M 228.1
Interatomic distances: F_5S—C 168.2, F_3S—C 139.2 pm; angle S—C≡S 180°. Formed from $CH_2(SF_3)_2$ + KOH at 80°. Colourless gas. Mp −130°. Dec. slowly above −78° and rapidly at r.t.

Gerhardt, R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1988, **27**, 1534 (*synth, F-19 nmr, ir, ms, cryst struct*)

IC-002439

CF_5NS_2

Pentafluoro(1,1,1-trifluoromethanesulfinimidoyl fluoridato-*N*)sulfur, 9Cl

[81912-70-1]

$F_3CS(F){=}NSF_5$

M 261.1
Synth. from NSF_3 + CF_3SF_3. Colourless liq. Bp 89°.

Lensch, C. *et al*, *Z. Naturforsch., B*, 1982, **37**, 306 (*synth, ir, ms, F-19 nmr*)

IC-002440

$CF_{10}N_2S_2$

Bis(pentafluorosulfur)carbodiimide

Decafluoro[μ-[methane diiminato(2−)-N:N']]disulfur, 11Cl

[58776-14-0]

$F_5SN{=}C{=}NSF_5$

M 294.1
From $F_5SNHC(O)NHSF_5$ + PCl_5 in CCl_4. Pale orange liq., not fully purif.

Thrasher, J.S. *et al*, *Inorg. Chem.*, 1982, **21**, 1616 (*synth, ir, ms*)

IC-002441

$CF_{12}FeOP_4$

Carbonyltetrakis(phosphorous trifluoride-*P*)iron, 9Cl

[16388-45-7]

$(F_3P)_4FeCO$

M 435.7
Pale-yellow liq. somewhat unstable towards H_2O and O_2. Sol. cyclohexane, C_6H_6, fluorocarbons, attacked rapidly by EtOH, Me_2CO. Stereochemically nonrigid.

Clark, R.J. *et al*, *Inorg. Chem.*, 1964, **3**, 1395 (*synth*)
Tripathi, J.B.P. *et al*, *J. Organomet. Chem.*, 1967, **9**, 307 (*synth, ir*)
Clark, R.J. *et al*, *Acc. Chem. Res.*, 1973, **6**, 246 (*rev*)
Mahnke, H. *et al*, *J. Chem. Phys.*, 1974, **60**, 2997 (*cmr, ir*)
Sheline, R.K. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1975, **14**, 314 (*ir, nmr*)
Sheline, R.K. *et al*, *New Synth. Methods*, 1975, **3**, 219 (*ir, nmr, synth*)
Head, R.A. *et al*, *J. Organomet. Chem.*, 1978, **145**, 75 (*pe*)

$CF_{12}OP_4Ru$

Carbonyltetrakis(phosphorous trifluoride)ruthenium, 9Cl IC-002442

Carbonyltetrakis(trifluorophosphine)ruthenium(0)

[36542-23-1]

$Ru(CO)(PF_3)_4$

M 480.9
May be a fluxional isomeric mixt. Isol. from the autoclave reaction of CO, PF_3 + $Ru_3(CO)_{12}$ at 150°. Yellow liq. ν_{CO} 2070, 2026 cm^{-1}.

Udovich, C.A. *et al*, *J. Organomet. Chem.*, 1972, **36**, 355 (*synth, nmr, ms*)

[CFe]

Iron carbides IC-002443

Iron carbides are of primary importance in Steel industry, particularly Fe_3C.

***Iron carbide* (Fe_3C)** [12011-67-5]
CFe_3 M 179.5
At low concentrations of C, steel comprises phases composed of Fe + Fe_3C. Dark grey air-sensitive powder. Mp 1250°.

Hexagonal-form: [12169-32-3]. ***Cementite***
CFe_3 M 179.5
Constituent of steel. Grey, cubic; pleated hexagonal array of Fe atoms; C in distorted trigonal prismatic sites. Mp 1837°. Dec. by dil. acid to form hydrocarbons. Curie point 210-215°; hard and brittle.

Mineral-form: [61027-57-4]. ***Cohenite***
CFe_3 M 179.5
Mineral, found in meteorites, volcanic rocks.

Solid soln.: [12244-31-4]. ***Austenite***
Formed >906° in smelting process; obt. by rapid quenching. Component of steel. Solid soln. of C in γ—Fe; C atoms arranged at random and in octahedral sites; (γ—Fe is fcc). Non-magnetic; adding Mn and Ni allows formation at lower temps. than when pure.

Solid soln.: [12173-93-2]. ***Martensite***
Obt. by quenching austenite below 150°. V. hard brittle steel (a characteristic property of quenched steels). Main use as a constit. of hardened carbon steel tools. A supersaturated solid soln. of C in α—Fe (bcc). Contains ≤1.6% C.

Solid soln.: [53469-19-5]. ***Sorbite*, 9Cl**
Formed by tempering martensite. Tougher steel than one formed by quenching. A mixt. of cementite (Fe_3C) and ferrite.

Solid soln.: [12427-27-9]. ***Pearlite***
From slow cooling (to 609°) of austenite. Eutectoid mixt. of cementite (Fe_3C) and ferrite; fine grain, soft steel.

Solid soln.: [12427-24-6]. ***Ferrite***
Occurs in steels, cast-iron, pig-iron. Almost pure α—Fe (bcc) with ≃0.06% C in solid soln.

***Iron carbide* (Fe_5C_2)** [12127-45-6]
C_2Fe_5 M 303.2
Originally formulated as Fe_2C. Struct. similar to cementite but with double layers of trigonal prismatic units; C is sited in prism. Curie point 248°.

***Iron carbide* (Fe_7C_3)** [12075-42-2]
C_3Fe_7 M 426.9
Curie point 250°.

***Iron carbide* (Fe_2C)** [12011-66-4]
ε-Fe_2C
CFe_2 M 123.7
Iron atoms are hcp.

[12173-11-4]

Bauer-Grosse, E. *et al*, *Wegliki, Azotki, Borti, Miedzynar. Konf., Irsk, 1984*, **45**; *CA*, **104**, 13298 (*Fe_3C, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, 1178.
Fasiska, E.J. *et al*, *Acta Crystallogr.*, 1965, **19**, 463 (*Fe_3C, struct*)
Nouveau Traité de Chimie Minérale, 1967, **XVII**, 830 (*bibl*)
Frad, W.A., *Adv. Inorg. Chem. Radiochem.*, 1968, **11**, 153 (*bibl*)
Le Caer, G. *et al*, *J. Solid State Chem.*, 1976, **19**, 19 (*Fe_3C, Fe_5C_2, mössbauer*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 499.
Kubaschewski, O., *Iron-Binary Phase Diagrams*, Springer, Berlin, 1982, 23 (*phase diagram*)
Yakel, H.L. *et al*, *Int. Met. Rev.*, 1985, **30**, 17 (*Fe_3C, struct, bibl*)
Kurmaev, E.Z. *et al*, *Carbon*, 1986, **24**, 249 (*Fe_3C*)

IC-002444

$CFeO_3$

Iron(*II*) carbonate ($FeCO_3$)

[563-71-3]

$FeCO_3$

M 115.8
Formed as white ppt. when Fe(*II*) solns. treated with alkali metal carbonate. Precursor for Fe(*II*) complexes and in diamond synth. Grey solid, dec. yielding CO_2 + FeO at 200°. Insol. H_2O, sol. acids to give CO_2; sol. H_2O saturated with CO_2 to give $Fe(HCO_3)_2$ which then oxidises.

Mineral-form
Siderite. *Chalybite. Spathic iron ore*
Ore widespread; may occur with some Ca, Mg or Mn. Yellow-brown to dark brown, or grey rhombohedral cryst. Dec. on heating.

Hydrate: Sl. sol. H_2O. Dec. on heating.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, **B2**, 502 (*bibl*)
Goldin, D.M. *et al*, *J. Therm. Anal.*, 1984, **29**, 139 (*thermal dec*)
Srivastava, K.K.P., *Phys. Rev. B*, 1985, **32**, 3282 (*mössbauer*)

[CGd]

IC-002445

Gadolinium carbides

Phases Gd_3C, Gd_2C_3, GdC_2 known.

***Gadolinium carbide* (GdC_2)** [12012-41-8]
C_2Gd M 181.2
Has CaC_2 struct. Brassy yellow solid. Dec. by H_2O. Undergoes α→β transition at 1218-1270°. μ_{eff} = 7.59μ_B (θ +41.3°); orders antiferromagnetically at 42K.

Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, magnetism*)
McColm, I.J. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1931 (*synth, props*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Male, G., *Rev. Int. Hautes Temp. Refract.*, 1977, **14**, 179; *CA*, 1978, **88**, 44271 (*synth*)
Sakai, T. *et al*, *J. Appl. Phys.*, 1979, **50**, 3592 (*magnetism*)

CHBrClF

IC-002446

Bromochlorofluoromethane

Fluorocarbon 21B1

[593-98-6]

$CHBrClF$

M 147.3

(+)-form [22611-58-1]
$[\alpha]_D^{19}$ +0.20° (c, 1.25 in cyclohexane). Opt. rotn. of opt. pure sample estimated to be ~3°.

(−)-form [31747-37-2]
$[\alpha]_{Hg}^{25}$ −0.13° (cyclohexane).

(±)-form [88987-26-2]
Liq. d_{15} 1.906. Fp −115°. Bp 36.5°.

Hazeldine, R.N., *J. Chem. Soc.*, 1952, 4259 (*synth*)
Hine, J. *et al*, *J. Am. Chem. Soc.*, 1958, **78**, 479 (*synth*)
Hargreaves, M.K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 16 (*synth*)
Hargreaves, M.K. *et al*, *J. Chem. Soc. C*, 1971, 1013 (*synth*)
Cancouil, J. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 6993 (*synth, resolu*)
Wilen, S.H. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 5997 (*resolu*)
Doyle, T.R. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 8510 (*resolu*)

$CHBrCl_2$

IC-002447

Bromodichloromethane, 9Cl

Dichloromethyl bromide. R 20B1. BDCM

[75-27-4]

Cl_2CHBr

M 163.8
Source of dichlorocarbene on treatment with base. d^{15} 2.056. Mp −57.1°. Bp 88.4-88.6° (89.2 - 90.6°).
▷ Mod. toxic by ingestion. PA5310000.

Seyferth, D. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 681 (*synth*)
Fedorynski, M. *et al*, *Synth. Commun.*, 1977, **7**, 287 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 564.

$CHBrF_2$

IC-002448

Bromodifluoromethane, 9Cl

Fluorocarbon 22B1

[1511-62-2]

$CHBrF_2$

M 130.9
$d_4^{15.7}$ 4.55. Bp −14.5°.

Swarts, F., *Bull. Acad. Roy. Med. Belg.*, 1910, 113 (*synth*)
Holzer, W. *et al*, *J. Mol. Spectrosc.*, 1968, **25**, 123 (*raman*)
Somayajulu, G.R. *et al*, *J. Magn. Reson.*, 1979, **33**, 559 (*cmr*)

$CHBr_2Cl$

IC-002449

Dibromochloromethane, 9Cl, 8Cl

Chlorodibromomethane. R 20B2

[124-48-1]

$CHBr_2Cl$

M 208.2
Source of bromochlorocarbene in the presence of base and crown ether. Liq. Fp −22°. Bp 121.3-121.8° (118-122°). n_D^{20} 1.5484.
▷ PA6360000.

Barrett, G.C. *et al*, *J. Chem. Soc. C*, 1971, 279 (*synth*)
Fedorynski, M. *et al*, *Synth. Commun.*, 1977, **7**, 287 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 795.

$CHBr_2F$

IC-002450

Dibromofluoromethane, 9Cl

Fluorocarbon 21B2

[1868-53-7]

Br_2CHF

M 191.8

Bromofluorocarbene source. Liq. d_4^{20} 2.42. Fp 26.5°. Bp 64.9°.

Urata, Y., *CA*, 1963, **59**, 5045 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1972, **3**, 77.
Andrews, L. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 3500 (*ir*)
Somayajulu, G.R. *et al*, *J. Magn. Reson.*, 1979, **33**, 559 (*cmr*)
Prochaska, F.T. *et al*, *J. Mol. Spectrosc.*, 1979, **76**, 142 (*ir*)

$CHBr_3$ IC-002451

Tribromomethane, 9CI
Bromoform. Methyl tribromide
[75-25-2]

$CHBr_3$

M 252.7
Synth. by bromination of Me_2CO or EtOH in the presence of base. Intermed. in org. synth., solvent for waxes, greases and oils. Heavy liq., non-flammable. d_4^{20} 2.887. Fp 9° (6-7°). Bp 150.3-151.2° (149.5°). Stabilised by addn. of 4% EtOH.

▷ Highly toxic vapour, irritant and lachrymatory, OES 5 mg m^{-3}. PB5600000.

Soroos, H. *et al*, *J. Am. Chem. Soc.*, 1945, **67**, 1642 (*synth*)
Kergomard, A., *Bull. Soc. Chim. Fr.*, 1961, 2360 (*synth*)
Kawaguchi, T. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 967 (*struct*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 210.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 568.

CHCdNOS IC-002452

Hydroxy(thiocyanato-*S*)cadmium(*II*)
[64700-57-8]

HOCdSCN

M 187.5
Cryst.
[53051-84-6]

Zuano Hernandez, G. *et al*, *An. Quim.*, 1974, **70**, 135; 1977, **73**, 820 (*synth, cryst struct*)
Pavlenko, V.A. *et al*, *Ukr. Khim. Zh.* (*Russ. Ed.*), 1985, **51**, 342 (*synth, ir*)

CHClFI IC-002453

Chlorofluoroiodomethane
[1512-28-3]

CHClFI

M 194.3
(±)-*form*
Light sensitive liq. Bp 76°, Bp_{150} 35°.

Hazeldine, R.N., *J. Chem. Soc.*, 1952, 4259 (*synth*)
Samajajulu, G.R. *et al*, *J. Magn. Reson.*, 1979, **33**, 559 (*C-13 nmr*)
Kudchadker, A.P. *et al*, *J. Phys. Chem. Ref. Data*, 1979, **8**, 499 (*props*)

$CHClF_2$ IC-002454

Chlorodifluoromethane
Fluorocarbon 22. Freon 22. Arcton 22
[75-45-6]

CHF_2Cl

M 86.4
Manuf. by reaction of $CHCl_3$ with anhydrous HF using antimony-based catalyst. Low-temp. refrigerant, intermed. for tetrafluoroethylene polymers, intermed. for fire-fighting agent ($CBrClF_2$). Gas. d_4^{-69} 1.49. Fp −160°. Bp −40.8°.

▷ Reacts exothermically with aluminium. Dec. to toxic carbonyl halides when heated strongly in air. OES 3500 mg m^{-3}. PA6390000.

Prosta, A. *et al*, *Chem. Listy*, 1957, **51**, 976 (*synth*)
Chalaye, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1967, **265**, 127 (*ir*)
San Filippo, J. *et al*, *J. Org. Chem.*, 1976, **41**, 392 (*nmr*)
Wheaton, G.A. *et al*, *J. Org. Chem.*, 1978, **43**, 2643 (*synth, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 60 (*use*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 242.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 802.

CHClOS IC-002455

Carbonochloridothioic acid, 9CI
Chlorothioformic acid, 8CI. Thiochloroformic acid
[16890-85-0]

$ClC(S)OH \rightleftharpoons ClC(O)SH$

M 96.5
Derivs. only known. Monochloride of Thiocarbonic acid, IC-002515. *O*-Derivs. are alkoxythiocarbonylating agents.

O-*Me:* [2812-72-8].
C_2H_3ClOS M 110.5
Bp 105-107°.

O-*Et:* [2812-73-9].
C_3H_5ClOS M 124.5
Bp_{40} 52-55°, Bp_{33} 46°.
▷ LQ6950000.

O-*Propyl:* [2812-74-0].
C_4H_7ClOS M 138.6
Bp_{12} 42°.

O-*Isopropyl:* [38363-18-7].
C_4H_7ClOS M 138.6
Bp_{10} 34° (Bp_4 35°).

O-*Butyl:* [2812-75-1].
C_5H_9ClOS M 152.6
Bp_{12} 62°.

O-tert-*Butyl:*
C_5H_9ClOS M 152.6
Bp_{10} 54°.

S-*Et:* [2941-64-2]. *Ethyl chlorothiolformate*
C_3H_5ClOS M 124.5
Reagent for synth. of *S*-esters. d_4^{20} 1.19. Bp 136°.
▷ Lachrymator, highly irritant.

S-*Propyl:* [13889-92-4].
C_4H_7ClOS M 138.6
Bp_{26} 59-60°.
▷ LQ7005000.

S-*Butyl:* [13889-94-6].
C_5H_9ClOS M 152.6
Bp 179°.

S-*Ph:* [13464-19-2].
C_7H_5ClOS M 172.6
Bp_{13} 104°.

Fieser and Fieser, Reagents for Organic Synthesis, **6**, 252.
Reimschneider, R. *et al*, *Monatsh. Chem.*, 1953, **84**, 518 (*synth*)
Tilles, H., *J. Am. Chem. Soc.*, 1959, **81**, 714 (*synth*)
Martin, D. *et al*, *Chem. Ber.*, 1965, **98**, 2059 (*synth, use*)
Berg-Neilsen, K. *et al*, *Acta Chem. Scand.*, 1972, **26**, 25 (*synth, pmr, ms*)
McKinnon, D.M. *et al*, *Can. J. Chem.*, 1972, **50**, 1401 (*props*)
Barany, G. *et al*, *J. Org. Chem.*, 1983, **48**, 4750 (*synth, props, bibl*)
Martínez, M. *et al*, *Synthesis*, 1986, 760 (*synth, ir, pmr, use*)

$CHClO_2S_2$ IC-002456

Chlorodisulfanylformic acid

Cl—S—S—COOH

M 144.6
Et ester:
$C_3H_5ClO_2S_2$ M 172.6
Yellow oily liq. $Bp_{0.4}$ 48°.
Chloride: [79341-73-4]. *Chloro chlorocarbonyl disulfide, 9CI. Chlorodisulfanylformyl chloride. 1-Chloro-2(chlorocarbonyl)disulfane*
CCl_2OS_2 M 163.0
Formed from $[(H_3C)_2CHOC(S)]_2S + SO_2Cl_2$ at 80° or from $ClCOS_3COCl + FeCl_3$. Yellow-orange liq. Bp_{12} 49°, Bp_{12} 53-54°.

Böhme, H. *et al*, *Justus Liebigs Ann. Chem.*, 1981, 1244.
Schroll, *et al*, *J. Org. Chem.*, 1986, **51**, 1866 (*synth, pmr*)

$CHCl_2F$ IC-002457

Dichlorofluoromethane, 9CI
Fluorocarbon 21
[75-43-4]

Cl_2CHF

M 102.9
Bacteriocide, refrigerant, solvent. Gas. d^9 1.405. Mp −135°. Bp 8.9°.

▷ Mod. toxic OES 40 mg m^{-3}. PA8400000.

Chalaye, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1967, **265**, 130 (*ir*)
Gilbert, R. *et al*, *J. Chem. Phys.*, 1974, **60**, 4820 (*ir*)
Ichikawa, M. *et al*, *CA*, 1976, **84**, 4444 (*synth*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 280.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1154.

$CHCl_2NO$ IC-002458

Hydroxycarbonimidic dichloride, 9CI
Phosgene oxime. Dichloroformaldoxime
[1794-86-1]

$Cl_2C{=}NOH$

M 113.9
Intermed. in heterocyclic synth. 1,3-Dipolar cycloaddition reagent. Mp 39-40°. Bp 129°. Sublimes on standing.

▷ Highly irritant. Highly toxic.

Prandtl, W. *et al*, *Ber.*, 1929, **62**, 1754, 2166; 1932, **65**, 754 (*synth*)
Birkenbach, L. *et al*, *Justus Liebigs Ann. Chem.*, 1931, **489**, 7 (*synth*)
Gryskiewicz-Trochimowski, E. *et al*, *Bull. Soc. Chim. Fr.*, 1948, 597 (*synth*)

Bravo, P. *et al*, *Gazz. Chim. Ital.*, 1961, **91**, 47 (*use*)
Halling, K. *et al*, *Justus Liebigs Ann. Chem.*, 1989, 985 (*synth, use*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 562.

$CHCl_2OPd^{\ominus}$ IC-002459

(Carbonyl)dichlorohydropalladate(1−)
Dichloro(carbonyl)palladate(1−) hydride. Hydridocarbonyldichloropalladate(1−)

$[PdCl_2H(CO)]^{\ominus}$

M 206.3 (ion)
Catalyses synth. of long-chained nitro compds.
Pyridinium salt: [25792-40-9].
$C_6H_7Cl_2NOPd$ M 286.4
Yellow solid, air-sensitive.
Quinolinium salt: [25870-10-4].
$C_{10}H_9Cl_2NOPd$ M 336.5
Yellow-green solid, air-sensitive.
Ph_4As salt: [25792-41-0].
Brown solid.

Kingston, J.V. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 455 (*synth, ir*)

$CHCl_2O_3Ta$ IC-002460

Dichloro(formato-*O,O'*)oxotantalum(*V*), 11CI
[88442-59-5]

$[TaOCl_2(OOCH)]_n$

M 312.8
Polymeric struct. of unknown geometry. Synth. by adding 2 mol. HCOOH to 1 mol. $TaCl_5$ in C_6H_6. White solid.

Viard, B. *et al*, *J. Chem. Res. (S)*, 1983, 252 (*synth, ir*)

$CHCl_3$ IC-002461

Chloroform
Trichloromethane, 9CI. R20
[67-66-3]

$CHCl_3$

M 119.3
Manuf. by direct chlorination of CH_4 or by reacn. of EtOH or Me_2CO with Cl_2 + NaOH. Solvent, intermediate for manuf. of $CHClF_2$, plastics intermediate. U.S. prodn. 136 000 t/a in 1976. Formerly used as anaesthetic. Used in the detection of phenols. Liq. Spar. sol. H_2O. d_4^{25} 1.481. Mp −63.2°. Bp 61.3°. n_D^{20} 1.4467. Nonflammable. Slowly dec. in air and light forming *inter alia* $COCl_2$ (toxic). Forms hydrate with $18H_2O$, dec. at 1.6°. Forms azeotrope contg. 2.5% H_2O, Bp 56°.

▷ Toxic vapour, OES 50 mg m^{-3}, eye irritant, suspected carcinogen. Vigorous reaction with Me_2CO and base, explosive reaction with some materials. FS9100000.

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 130; **8**, 92.
Dykes, M.H.M., *Int. Anesthesiol. Clin.*, 1970, **8**, 357 (*rev, pharmacol*)
Legradi, L., *Mikrochim. Acta*, 1972, 369 (*use*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 693 (*rev*)
Davidson, I.W.F. *et al*, *Drug Chem. Toxicol.*, 1982, **5**, 87 (*rev, metab, tox*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 3104.
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.

Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 245.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 828.

IC-002482

$CHCl_4NNb$

Pentachloro(hydrocyanic acid)niobium(*V*), 9Cl
Pentachloro(hydrogen cyanide)niobium(V).
Pentachloro(formonitrile)niobium(V)
[36349-63-4]

$(HCN)NbCl_5$

M 297.1
Octahedral; the N—C bond is shorter than that in free HCN. Synth. by dissolving freshly sublimed $NbCl_5$ in anhydrous HCN at 50°. Colourless, air- and heat-sensitive solid.
▷ Cyanides are toxic.
Clarani, C. et al, Acta Crystallogr., Sect. B, 1975, 31, 1823 (synth, cryst struct)

IC-002483

$CHCsO_3$

Caesium hydrogen carbonate ($CsHCO_3$)
Caesium bicarbonate. Carbonic acid, monocaesium salt, 8Cl.
Caesium carbonate (1:1)
[29703-01-3]

$CsHCO_3$

M 193.9
Prepd. by treatment of aq. Cs_2CO_3 with CO_2.
Commercially available. Colourless monoclinic cryst; dec. at 175° with H_2O and CO_2 loss. V. sol. H_2O (209 g per 100 cm^3 at 15°). Sol. EtOH. ΔH_f° −966 kJ mol^{-1}; ΔG_f° −832 kJ mol^{-1}; S° 130 J K^{-1} mol^{-1}.
Sigma-Aldrich Library of Chemical Safety Data 1988, 2, 715B
Gmelin Handbook Inorg. Chem., Syst. No. 25, 1935, 236 (rev., bibl)
Cameron, C. et al, J. Appl. Crystallogr., 1972, 5, 248; CA, 77, 40184 (cryst struct)

IC-002484

$CHFO_2$

Fluoroformic acid, 8Cl
Carbonofluoridic acid, 8Cl
[1538-06-3]

FCOOH

M 64.0
Me ester:
$C_2H_3FO_2$ M 78.0
Liq. Mp 39-40°.
▷ Highly irritant. Evolves HF on contact with H_2O
tert-Butyl ester:
$C_5H_9FO_2$ M 120.1
Reagent for amino acid protection. Liq. Bp 79-80°, Bp_{15} 40-42°.
Ph ester: [351-80-4]
$C_7H_5FO_2$ M 140.1
Bp_{15} 60-63°.
Benzyl ester: [93942-41-7].
$C_8H_7FO_2$ M 154.1
Liq. Bp 44-46°.
Isopropyl: [461-71-2].
$C_4H_7FO_2$ M 106.0
Et: [461-64-3]
$C_3H_5FO_2$ M 92.0
Nitrile: see Cyanogen fluoride, C-20257
Tullock, C.W. et al, J. Org. Chem., 1960, 25, 2016 (synth)

Neimysheva, A.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1967, 177, 856 (*nmr*)
Schnabel, E. *et al*, *Justus Liebigs Ann. Chem.*, 1968, 716, 175 (*synth, use*)
Carpino, L.A. *et al*, *J. Org. Chem.*, 1970, **35**, 3291 (*synth*)
William, G. *et al*, *Trans. Faraday Soc.*, 1971, **67**, 950 (*ir*)
Cuomo, J. *et al*, *J. Org. Chem.*, 1979, **44**, 1016 (*synth*)
Olah, G.A. *et al*, *J. Org. Chem.*, 1979, **44**, 3872 (*synth*)
Dang, V.A. *et al*, *J. Org. Chem.*, 1990, **55**, 1847 (*synth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 821.

CHF_2N

Carbonimidic difluoride, 9Cl IC-002485
Difluoromethanimine
[2712-98-3]

$F_2C{=}NH$

M 65.0
Reported syntheses prior to 1988 were erroneous. Synth. from F_3CNH_2 in Et_3N at −78° or from F_3CNCO + H_2O/Et_3N. Gas. Mp −90 to −89°. Stable < −13° or at < 5mm pressure. Dec. to CF_3NH_2 + FCN.
Bürger, H. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 105 (*synth, F-19 nmr, ir, raman*)

CHF_3

Trifluoromethane, 9Cl, 8Cl IC-002488
Fluoroform. Fluorocarbon 23. Carbon trifluoride
[75-46-7]

CHF_3

M 70.0
Refrigerant for low temps., intermed. for org. synth. Odourless gas. Sol. H_2O. d^{-100} 1.52. Mp −163°. Bp −82.1°. Bp 20° at 40 atm.
▷ Low toxicity, narcotic in high concentration. PB6900000.
Henne, A.L., *J. Am. Chem. Soc.*, 1937, **59**, 1200 (*synth*)
Gol'dfarb, L.V. *et al*, *CA*, 1971, **75**, 26815 (*ms*)
Moss, J.H. *et al*, *J. Fluorine Chem.*, 1975, **6**, 393 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 717.

CHF_3OS

IC-002487

Trifluoromethanesulfenic acid, 9Cl
[306-79-6]

F_3CSOH

M 118.0
Me ester: [1544-50-9]. *Methyl trifluoromethanesulfenate*
$C_2H_3F_3OS$ M 132.1
Liq. Bp 25-26°.
Et ester: [691-04-3]. *Ethyl trifluoromethanesulfenate*
$C_3H_5F_3OS$ M 146.1
Liq. Bp 47-49°.
2,2,2-Trifluoroethyl ester: Liq. Bp 44-50°.
Isopropyl ester
$C_4H_7F_3OS$ M 160.1
Liq. Bp 68-70°.
Hasszeldine, R.N. *et al*, *J. Chem. Soc.*, 1955, 2901.

CHF_3O_3S

IC-002488

Trifluoromethanesulfonic acid, 11Cl, 9Cl
Triflic acid
[1493-13-6]

F_3CSO_3H

M 150.0
Catalyst for isomerisations, alkylations etc. Liq. Misc. H_2O. d_4^{20} 1.69. Bp 162°. Fumes in moist air; very hygroscopic, forming monohydrate, Mp 34°. Very strong acid.
Na salt: [2926-30-9].
Solid. Mp 251°.
Me ester: [333-27-7].
$C_2H_3F_3O_3S$ M 164.1
Important reagent for methylations. d_4^{20} 1.45. Bp 99°.
▷ Corrosive, severe poison.
Et ester: [425-75-2].
$C_3H_5F_3O_3S$ M 178.1
Bp 115°.
Trifluoromethyl ester: [3582-05-6]. *Trifluoromethyl trifluoromethanesulfonate*
$C_2F_6O_3S$ M 218.0
Trifluoromethylating agent. Liq.
Trimethylsilyl ester: see *Trimethylsilyl trifluoromethanesulfonate, IC-004115*
Fluoride: [335-05-7].
CF_4O_2S M 152.0
Gas. Bp −21.7°. Hydrol. by H_2O only v. slowly at r.t., slowly at 100°.
Chloride: [421-83-0].
$CClF_3O_2S$ M 168.5
Bp 31.6°.
Anhydride: [358-23-6].
$C_2F_6O_5S_2$ M 282.1
Reagent for synth. of triflates and dehydration of aldoximes. Bp 84°.
Amide: [421-85-2].
$CH_2F_3NO_2S$ M 149.0
Mp 117-118°.
Diethylamide: [28048-17-1].
$C_5H_{10}F_3NO_2S$ M 177.1
Bp, 55°.

Hasszeldine, R.N. *et al*, *J. Chem. Soc.*, 1954, 4228 (*synth*)
Gramstad, T. *et al*, *J. Chem. Soc.*, 1956, 173 (*deriv*)
Burdon, J. *et al*, *J. Chem. Soc.*, 1957, 2574 (*synth*)
Robinson, E.A., *Can. J. Chem.*, 1961, **39**, 247 (*ir*)
Baird, C.D. *et al*, *J. Org. Chem.*, 1973, **38**, 3673 (*synth*)
Howells, R.D. *et al*, *Chem. Rev.*, 1977, **77**, 69 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 406; 1979, **7**, 390.
Forbus, T.R. *et al*, *J. Org. Chem.*, 1979, **44**, 313; 1987, **52**, 4156 (*deriv*)
Taylor, S.L. *et al*, *J. Org. Chem.*, 1987, **52**, 4147 (*deriv, synth, use, bibl*)
Tordeux, M. *et al*, *J. Org. Chem.*, 1989, **54**, 2452 (*synth, F-19 nmr*)

CHI_3

IC-002489

Triiodomethane, 9Cl, 8Cl
Iodoform
[75-47-8]

CHI_3

M 393.7
Produced by *Aspergillus oxydans*. Powerful antiseptic, disinfectant. Commercially available. Yellow hexagonal plates (Me_2CO), with characteristic disagreeable odour. Sol. org. solvs., pract. insol. H_2O. d_4^{20} 4.1. Mp 119-120°. Dec. slowly in light, steam-volatile.
▷ Toxic, TLV 10. PB7000000.
Datta, R.L. *et al*, *J. Am. Chem. Soc.*, 1917, **39**, 441 (*synth*)
Seelye, R.N. *et al*, *J. Chem. Educ.*, 1959, **36**, 572 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 266.
Iwata, Y. *et al*, *CA*, 1976, **85**, 54017 (*cryst struct*)
Burrows, B.J. *et al*, *J. Agric. Food Chem.*, 1978, **26**, 856 (*anal, rev, pmr*)
Anders, M.W. *et al*, *Drug Metab. Dispos.*, 1978, **6**, 556 (*metab*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 457?
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 365.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1988.

$CHKO_2$

IC-002470

Potassium formate
Formic acid, potassium salt, 8Cl. Methanoic acid, potassium salt
[590-29-4]

K(OOCH)

M 84.1
Synth. by dissolving K_2CO_3 in aq. formic acid. Commercially available. Deliquescent colourless orthorhombic cryst. Dec. on heating forming $K_2C_2O_4$ as intermed. and K_2CO_3 as final product. V. sol. H_2O (331 g per 100 cm^3 at 18°; 657 g per 100 cm^3 at 80°); sol. EtOH; insol. Et_2O. Mp 165-168°.
▷ Irritant. LQ9625000.
Harvey, K.B. *et al*, *Can. J. Chem.*, 1963, **41**, 1181 (*ir*)
Braghetti, M. *et al*, *Riv. Sci.*, 1969, **39**, 576 (*thermodec*)
Barraldi, P., *Spectrochim. Acta, Part A*, 1970, **35**, 1063 (*ir, thermal dec*)
Batts, J.W. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1940 (*cryst struct*)
Mentzen, B.F. *et al*, *Inorg. Chim. Acta*, 1980, **43**, 237 (*cryst struct*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1716A (*haz*)

$CHKO_3$

IC-002471

Potassium hydrogen carbonate ($KHCO_3$)
Potassium bicarbonate. Potassium carbonate (KHCO3). Carbonic acid, monopotassium salt, 8Cl
[298-14-6]

$K[HCO_3]$

M 100.1
Synth. by bubbling CO_2 through an aq. soln. of K_2CO_3. Commercially available. Coal gasification catalyst. Buffer in H_2O treatment and wine production. Constit. of effervescent pharmaceutical preps. Colourless monoclinic cryst. Hygroscopic. Dec. on heating with H_2O and CO_2 loss. V. sol. H_2O (50 g per 100 cm^3 at 60°); insol. EtOH. ΔH_f° −963 kJ mol^{-1}; ΔG_f° −864 kJ mol^{-1}; S° 116 J K^{-1} mol^{-1}.
Lucenante, C., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1940, **229**, 1215 (*comput*)
Nitta, I. *et al*, *Acta Crystallogr.*, 1954, **7**, 140 (*cryst struct*)
Zhabrova, G.M. *et al*, *Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1959, 946; *CA*, 1960, **54**, 36 (*abs*)

Novak, A. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1385 (*ir*)
Feucht, H. *et al*, *Z. Naturforsch., A*, 1976, **31**, 1173 (*pmr*)

IC-002472

CHLiO$_2$

Lithium formate
Lithium methanoate. Formic acid, lithium salt, 8CI. Methanoic acid, lithium salt
[556-63-8]

LiOOCH

M 51.9
Prepared by neutralisation of Li_2CO_3 by formic acid; cryst. as monohydrate. Dec. at 230°.
Monohydrate: [6108-23-2].
CH_3LiO_3 M 69.9
Piezoelectric. White orthorhombic cryst. dec. on heating by H_2O loss (−H_2O at 94°). V. sol. H_2O (28g per 100 cm^3 at 18°; 57g per 100 cm^3 at 98°); spar. sol. EtOH, Me_2CO; insol. C_6H_6.
Nitta, A., *Sci. Pap. Inst. Phys. Chem. Res. (Jpn.)*, 1928, **9**, 151 (*monohydrate, cryst struct*)
Duval, C. *et al*, *Ann. Phys.*, 1942, **17**, 5 (*ir, monohydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 505 (*rev, bibl, monohydrate*)
Harvey, K.B. *et al*, *Can. J. Chem.*, 1963, **41**, 1381 (*ir*)
Donaldson, J.D. *et al*, *Spectrochim. Acta*, 1964, **20**, 847 (*ir, struct*)
Grigor'ev, A.I., *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1966, **171**, 126 (*ir*)
Muthukrishnan, K. *et al*, *CA*, 1973, **78**, 152555 (*pmr, monohydrate*)
Hashizume, S. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 3971 (*cryst struct*)
Yurzak, V. *et al*, *Kristallografiya*, 1977, **22**, 106 (*Li-7 nmr*)
Agarwal, A. *et al*, *Can. J. Chem.*, 1983, **61**, 2282 (*ir, raman, monohydrate*)

CHN

IC-002473

Hydrocyanic acid, 11Cl, 9Cl
Hydrogen cyanide. Prussic acid. Formonitrile
[74-90-8]

HC≡N (C_{2v})

M 27.0
Interatomic distances: H—C 106.55, C—N 115.32 pm. Constit. of apricot kernels (1.4 mg g^{-1}), present in tobacco smoke. Formed from NaCN and H_2SO_4. Gas used for exterminating rodents in ships, insects on trees, etc. Reagent used in Gattermann aldehyde synth. and for synth. of amino acids. Used in manuf. of methacrylates and methionine. Commercially available. Extensive uses in org. synth. V. volatile liq. or colourless gas smelling of bitter almonds. Misc. H_2O, EtOH, Et_2O. d^0 0.715. Mp −13°. Bp 25.7°. pK_a 9.89. Aq. solns. are unstable. Burns with violet flame. V. weak acid. Can condense to a tetramer or a black polymer. T_{ext} 183.5°.
▷ V. toxic, fatal dose *ca.* 60 mg. Extremely flammable, flash p. −18°. MW6825000.
[26746-21-4, 91280-07-8]
Org. Synth., Coll. Vol., 1, 1932, 314 (*synth*)
Andrussow, *Angew. Chem.*, 1935, **48**, 593 (*synth*)
Wintersteiger, G. *et al*, *J. Mol. Spectrosc.*, 1971, **39**, 149 (*struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 252.
Sastry, G.R.N., *Indian J. Chem.*, 1975, **10**, 33 (*rev*)
Brauer, G., *Handbuch Prap. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 628 (*synth*)
Weigert, W. *et al*, *CA*, 1978, **89**, 45705n (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **7**, 307 (*rev*)

Pesticide Manual, 6th Ed., 1979, 300 (*use*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 290.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 354.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1904.

CHNO

IC-002474

Cyanic acid, 11Cl
Hydrogen cyanate
[420-05-3]

HOC≡N

M 43.0
Is not in equilib. with Isocyanic acid, IC-002476. Refs. are freq. confused in CA. Obt. in Ar matrix. Kinetically unstable. Formed by dist. of cyanuric acid. pK_a 3.46.
Jacox, M.E. *et al*, *J. Chem. Phys.*, 1964, **40**, 2457.
Groving, N. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1768 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 170.
Brauer, G., *Handbuch Prap. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 634 (*synth*)
Bondybey, V.E. *et al*, *J. Mol. Spectrosc.*, 1982, **92**, 431.
Teles, J.H. *et al*, *Chem. Ber.*, 1989, **122**, 753 (*struct, bibl*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 526.

CHNO

IC-002475

Fulminic acid, 9Cl, 8Cl
Carbyloxime. Hydrogen cyanide-N-oxide
[506-85-4]

HC≡N$^{\oplus}$—O$^{\ominus}$ ($C_{\infty v}$)

M 43.0
Has the struct. shown rather than C$^{\ominus}$≡N$^{\oplus}$OH which was prev. postulated. Interatomic distances H—C 102.7, C—N 116.8, N—O 119.9 pm. The free acid is stable for a time only in Et_2O soln. at low temps.; it polymerises rapidly. Metal salts are widely used in detonators.
▷ Salts highly explosive, shock-sensitive, Hg salt is highly toxic. LS9320000.
Trimolecular Me ester:
C_3H_3NO M 57.0
Needles (H_2O). Mp 149°.
Deutero compd: [20411-64-7]. *Fulminic acid*-d.
Deuterofulminic acid
CDNO M 44.0
Synth. from HCNO + D_2O in vapour phase or Hg fulminate + D_2O + Na/Hg.
[51060-05-0]
Wieland, H., *Ber.*, 1910, **43**, 3362 (*synth*)
Wöhler, L. *et al*, *Ber.*, 1929, **62**, 2742, 2748 (*salts*)
Bodensch, H.K. *et al*, *Z. Naturforsch., A*, 1969, **24**, 1973 (*synth, struct, deutero, deriv*)
Beck, W. *et al*, *Chem. Ber.*, 1971, **104**, 533 (*ir, struct*)
Grundmann, C. *et al*, *Justus Liebigs Ann. Chem.*, 1973, 898.
Rodd's Chem. Carbon Compd. (*2nd Ed.*), 2nd Ed., 1973, 143 (*rev*)
Wentrup, C. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1979, **91**, 503 (*synth*)
Bondybey, V.E., *J. Mol. Spectrosc.*, 1982, **92**, 431 (*synth, uv-vis, deutero, deriv, photol, isom*)
De Sarlo, F. *et al*, *Tetrahedron*, 1985, **41**, 5181 (*synth, prepn*)
Teles, J.H. *et al*, *Chem. Ber.*, 1989, **122**, 753 (*struct, bibl*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 276, 405.

Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 383, 471.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1776.

CHNO

IC-002476

Isocyanic acid, 8Cl
[75-13-8]

HN=C=O

M 43.0
Contrary to popular belief, is not in equilib. with Cyanic acid, IC-002474. Freq. confused with cyanic acid in 9CI. Interatomic distances: H—N 98.6, N—C 120.9, C—O 116.6 pm; angle HNC 128°. Formed by thermal dec. of trimer $(HNCO)_3$. Reagent for conversion of alcohols to allophanates. Also adds to carbonyl compds. and alkenes. Liq. or gas with strongly acrid odour. d^0 1.140. Mp −86°. Bp 23.5°. pK_a 3.66.
▷ Lachrymator, vesicant, highly toxic.
Deutero derin.: [10357-59-2]. *Isocyanic acid*-d. *Deutero isocyanic acid*
CDNO M 44.0
Formed by photolysis of CD_3NO_2 or cyanuric acid + D_2O followed by pyrolysis. Identified in Ar matrix.
v. Dohlen, W.C. *et al*, *Acta Crystallogr.*, 1955, **8**, 646 (*struct, synth, ir*)
Steyermark, P.R., *J. Org. Chem.*, 1963, **28**, 586 (*synth*)
Groving, N. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1768 (*synth*)
Boughton, J.H. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 2851 (*diss const*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 170.
Inorg. Synth., 1972, **13**, 17 (*synth*)
Hocking, W.H. *et al*, *Can. J. Phys.*, 1975, **53**, 1869 (*struct*)
Sengodan, V. *et al*, *Indian J. Pure Appl. Phys.*, 1981, **19**, 1824 (*deutero derin, struct*)
Belson, D.J. *et al*, *Chem. Soc. Rev.*, 1982, **11**, 41 (*rev*)
Bondybey, V.E. *et al*, *J. Mol. Spectrosc.*, 1982, **92**, 431 (*synth, spectrum, isom, photol*)
Jacox, M.E., *J. Phys. Chem.*, 1984, **88**, 3373 (*synth, deutero deriv*)
Teles, J.H. *et al*, *Chem. Ber.*, 1989, **122**, 753 (*struct, bibl*)

CHNO

IC-002477

Isofulminic acid

HO—N$^{\oplus}$≡C$^{\ominus}$

M 43.0
Calc. as intermed. in stability between fulminic and isocyanic acids. Intermed. in the thermal or photochem. dec. of $HCON_3$.
Rauk, A. *et al*, *Can. J. Chem.*, 1977, **55**, 1498 (*theory*)
Benedetti, P.G. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1982, 95 (*org reactions*)
Yoshimura, Y. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 5414 (*org reactions*)

CHNS

IC-002478

Isothiocyanic acid
[3129-90-6]

HN=C=S (C_s)

M 59.0
Interatomic distances: H—N 98.9, N—C 121.6, C—S 156.1 pm; angle: HNC 135°. pK_a 0.97.
▷ NX8210000.

CHNS

IC-002479

Thiocyanic acid, 9Cl
Sulfocyanic acid. Hydrogen thiocyanate
[463-56-9]

HSC≡N

M 59.0
V. strong acid. Present in Cruciferae e.g. *Brassica* spp. Synth. from KNCS + $KHSO_4$. Polymerises at −90°, stable in dil. aq. soln. Sol. H_2O, EtOH, Et_2O. Mp −110°. pK_a −1.85 (25°).
Me ester: [556-64-9]. *Methyl thiocyanate*
C_2H_3NS M 73.1
Liq. d^{15} 1.077. Fp −91°. Bp_{98} 130.5°. n_D^{15} 1.0765.
Et ester: [542-90-5]. *Ethyl thiocyanate, 9CI*
C_3H_5NS M 87.1
Liq. Insol. H_2O. d^{18} 1.020. Bp 146°.
Propyl ester: [4251-16-5].
C_4H_7NS M 101.1
Liq. with unpleasant odour. Bp 163°.
Allyl ester: Allyl thiocyanate
C_4H_5NS M 99.1
Bp 161°.
▷ Highly toxic.
Ph ester: [5285-87-0].
C_7H_5NS M 135.1
Bp 231°.
▷ XL1850000.
Kaufmann, H.P., *Ber.*, 1926, **59**, 187 (*synth*)
Dienske, J.W., *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1927, **46**, 154.
Allen, P., *J. Am. Chem. Soc.*, 1935, **57**, 198 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 366 (*synth*)
Brintzinger, H. *et al*, *Chem. Ber.*, 1952, **85**, 455 (*synth, Me ester*)
Gmelin, R. *et al*, *Acta Chem. Scand.*, 1960, **14**, 507 (*ssl, biosynth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 954.
Emerson, D.W., *J. Chem. Educ.*, 1971, **48**, 81 (*synth*)
Harpp, D.N. *et al*, *Synthesis*, 1979, 181 (*synth, Me ester*)
Knoke, D. *et al*, *Pharmazie*, 1973, **28**, 574, 617 (*rev, synth, Me ester*)
Newman, A.A., *Chem. Biochem. Thiocyanic Acid and its Derivs.*, 1975, 1975 (*rev*)
Brauer, G., *Handbuch Prap. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 635 (*synth*)
Reeves, W.P. *et al*, *Synth. Commun.*, 1976, **6**, 509 (*synth, Et ester*)
Katritzky, A.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 133 (*synth, Et ester*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **22**, 156.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2395, 3257.

CHNSe

IC-002480

Isoselenocyanic acid
[71048-67-4]

HN=C=Se

M 105.9
From AgNCSe + HBr. Identified by its microwave spectrum. $t_{\frac{1}{2}}$ 90s in a microwave cell at 0.01 mm.
Ag salt:
CAgNSe M 212.8
Landsberg, B.M., *Chem. Phys. Lett.*, 1979, **60**, 265 (*struct*)

CHNSe IC-002481

Selenocyanic acid

[3085-11-2]

HSeC≡N

M 105.9

Unstable as free acid. From KSeCN + H^+ pK_a <1 (25°).

K salt: see Potassium selenocyanate, IC-002732

Boughton, I.B. *et al. J. Inorg. Nucl. Chem.*, 1968, **28**, 2851 (pK_a)

CHNTe IC-002482

Tellurocyanic acid

[66307-00-6]

HTeC≡N

M 154.6

Unstable as the free acid. Formed from Te + KCN in DMSO, as the K salt. Dec. in air or H_2O (as the anion).

K salt: [75457-69-1]

CKNTe M 192.7

Spencer, H.K. *et al. J. Am. Chem. Soc.*, 1977, **99**, 1470 (synth, *K salt*)

CHN_3S_3 IC-002483

1,3,5,2,4,6-Trithiatriazapine

M 151.2

Highly volatile plates (pet. ether). Mp 43°.

Dunn, P.J. *et al. J. Chem. Soc., Perkin Trans. 1*, 1988, 1745 (synth *as 1,3,5,2,4,6-trithiatriazepine*, struct, mol)

$CHNaO_2$ IC-002484

Sodium formate

Formic acid, sodium salt. HCI. Methanoic acid, sodium salt

[141-53-7]

Na(OOCH)

M 68.0

Manuf. from CO and either NaOH or $NaHCO_3$. Also produced by reaction of CO_2 with sodium amalgam in aq. soln. Commercially available. Reducing agent widely used in org. chem. Stabilising agent particularly for enzyme containing liq. detergents. Colourless monoclinic deliquescent cryst. V. sol. H_2O (97g per 100cm³ at 20°, 160g per 100cm³ at 100°); spar. sol. EtOH; insol. Et_2O. Mp 259-261°, ΔH° −649 kJ mol⁻¹. Dec. on heating with evolution of CO and H_2 and formation of $Na_2C_2O_4$ and Na_2CO_3 (300-400°).

▷ Irritant: LR0150000.

Newman, R., *J. Chem. Phys.*, 1952, **20**, 1683 (*s*)

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1398 (rev, *ref*)

Bjerrum, E., *J. Chem. Soc. B*, 1967, 879 (*s*; *vapour*)

Rudolph, R., *J. Prakt. Chem.*, 1971, **312**, 887; *C.A.*, **74**, 118119 (*pmr*)

Markila, P.L. *et al. Acta Crystallogr., Sect. B*, 1975, **31**, 2927 (*cryst struct*)

Tahara, R. *et al. Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1736C (*haz*)

$CHNaO_3$ IC-002485

Sodium hydrogen carbonate

Sodium bicarbonate. Carbonic acid, monosodium salt. HCI. Baking soda

[144-55-8]

$NaHCO_3$

M 84.0

Manuf. by the Solvay process when CO_2 is passed into ammoniacal brine. Also prod. either by treatment of aq. Na_2CO_3 with CO_2 or by dissolution of trona in H_2O saturated with CO_2. Commercially available. Blowing agent, foaming agent, food additive. Component of photographic developers. Constit. of effervescent pharmaceutical preps. and powder fire extinguishers. White monoclinic cryst. or powder. Dec. on heating → CO_2, H_2O and Na_2CO_3. Mod. sol. H_2O (6.9 g per 100 cm³ at 0°; 16 g per 100 cm³ at 60°); spar. sol. EtOH. ΔH_f° −951 kJ mol⁻¹; ΔG_f° −851 kJ mol⁻¹; S° 102 J K⁻¹ mol⁻¹.

▷ VZ0950000.

Sass, R.L. *et al. Acta Crystallogr.*, 1962, **15**, 77 (*cryst struct*)

Nowak, A. *et al. J. Chim. Phys. Phys.-Chim. Biol.*, 1965, **62**, 1301 (*pr*)

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **18**, 458 (*rev, uses*)

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 267; 1967, **3**, 1349 (*rev, bibl*)

Davies, J. *et al. Trans. Faraday Soc.*, 1971, **67**, 3463 (*pmr*)

Tabata, R. *et al. Bull. Chem. Soc. Jpn.*, 1986, **59**, 1951 (*Na-23 nmr*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1140A (*haz*)

CHO_2Tl IC-002486

Thallium(*I*) formate

Thallium(I) methanoate

[992-98-3]

TlOOCH

M 249.4

Orthorhombic; Tl in trigonal bipyramidal environment with the Tl atom occupying one apex of the eq. plane and each formate ion bridging two Tl atms. Tetramers in soln. Obt. by reaction of Tl_2CO_3 or TlOH with formic acid. Used extensively in org. synth. Heavy liq. for gravity conc. of ores. Hygroscopic colourless light-stable cryst. (MeOH). V. sol. H_2O; mod. sol. MeOH; spar. sol. EtOH. Mp 101°

▷ V. toxic.

Tetramer: Tetrakis(formato)tetrathallium

$C_4H_4O_8Tl_4$ M 997.6

Taylor, E.C. *et al. Acc. Chem. Res.*, 1970, **3**, 338 (*reactions*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 887 (*synth*)

Oddon, Y. *et al. Inorg. Chim. Acta*, 1981, **48**, 129 (*struct*)

Comprr. Organomet. Chem., Pergamon, Oxford, 1982, **7**, 467 (*reactions*)

Ozutsumi, K. *et al. Bull. Chem. Soc. Jpn.*, 1984, **57**, 2612 (*struct, soln*)

CHO_3Rb IC-002487

Rubidium hydrogen carbonate

Rubidium bicarbonate. Carbonic acid, monorubidium salt. HCI

[19088-74-5]

$Rb(HCO_3)$

M 146.4

Struct. contains planar CO_3 units linked by H-bonds into dimers. Prepd. by treatment of an aq. soln. of Rb_2CO_3 with CO_2. Colourless monoclinic cryst. Dec. on heating with H_2O loss and CO_2 loss. V. sol. H_2O (54 g per 100 cm³ at 20°); sol. EtOH. ΔH_f° −963 kJ mol⁻¹; ΔG_f° −864 kJmol⁻¹; S° 121 J K⁻¹ mol⁻¹.

Gmelin Handbook Inorg. Chem., Syst. No. 24, 1955, 224 (*rev, bibl*)

Le Naour, A. *et al. J. Chim. Phys. Phys.-Chim. Biol.*, 1967, **64**, 1643 (*pr*)

Kim, M.J., *Taehan Hwahakhhoe Chi.*, 1968, **13**, 131; *C.A.*, 1970, **72**, 16586 (*cryst struct*)

[CHTi] IC-002488

Titanium carbide hydride, 11Cl

[11130-17-9]

TiC_xH_y $0.55 \leqslant x \leqslant 0.7$, $0.14 \leqslant y \leqslant 0.26$

Both ordered and disordered phases based on $TiC_{0.75}$ are known. H is in octahedral holes. Synth. by heating $TiC_{0.75}$ in H_2.

Lazarguin, I.S. *et al. Izv. Akad. Nauk SSSR Neorg. Mat.*, 1984, **20**, 1948 (*synth, cryst struct*)

Lazarguin, I.S. *et al. Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1985, 25 (*synth, cryst struct*)

CH_2AlNaO_3 IC-002489

Dihydroxyaluminium sodium carbonate, USAN

[Carbonato(2−)-O,O′]dihydroxyaluminate(1−) sodium. Carbaldrate, INN. Dawsonite. Kompensan. Mimicid. Neucid. Rolaids

[4342-54-5]

$(HO)_2AlNaCO_3$

M 143.9

Synth. from aluminium alkoxide + $NaHCO_3$ in H_2O. Antacid. Amorph. powder + xH_2O or poorly formed cryst.

[2011-77-7, 16482-55-6, 41342-54-5]

Gunn, J.W. *et al. J. Am. Pharm. Assoc.*, 1955, **44**, 219 (*synth, prop*)

U.S. Pat., 2 783 179, (1957); *C.A.*, **51**, 10009g (*synth*)

Kroschwitz, J.C., *Kirk-Othmer Encycl. Chem. Technol.*, 2nd Ed., Wiley, N.Y., 1963-1971, **2**, 427 (*rev*)

Gazzaniga, E., *Chem. Eng. (N.Y.)*, 1965, **72**, 168 (*synth, prop*)

Serra, C.J. *et al. J. Pharm. Sci.*, 1978, **67**, 324 (*cryst struct*)

Palida, R. *et al. Sci. Pharm.*, 1979, **47**, 181 (*synth, ir*)

Keenan, F.J., *Diss. Abstr. Int., B*, 1982, **42**, 3255 (*synth, struct*)

Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 689

CH_2BN IC-002490

Cyanoborane

Boranecarbonitrile. HCI. 9CI

[6633-76-5]

$[BH_2CN]_n$

M 38.8

Forms homopolymer. Prepd. from $NaBH_3CN$ in Et_2O by addition of HCl gas. Air- and moisture-sensitive white semi-solid. Sol. HMPA, CH_2Cl_2. Ir 2469, 2441, 2429, 2295 cm⁻¹ (neat).

4-Methylaniline complex: [66632-45-9]. *(Cyano-C)dihydro(4-methylbenzenamine)boron, HCI. Boranecarbonitrile compd. with 4-methylbenzenamine (1:1). Cyanoborane p-toluidine*

$C_8H_{11}BN_2$ M 145.9

White cryst. (THF/pet. ether). Mp 134°.

Bhattacharjee, A. *et al. Tetrahedron Lett.*, 1972, 3173 (*synth*)

Vidal, J.C. *et al. Inorg. Chem.*, 1977, **16**, 1890 (*synth, prop*)

Hutchins, R.O. *et al. J. Org. Chem.*, 1977, **42**, 82 (*synth, r, uses*)

Wiman-Nellsson, P. *et al. Inorg. Chem.*, 1978, **17**, 2027 (*deriv, synth, pmr, ir*)

Martin, D.R. *et al. J. Inorg. Nucl. Chem.*, 1978, **40**, 9 (*synth, use*)

Compr. Org. Chem., Pergamon, Oxford, 1979, **3**, 695 (*rev*)

$CH_2Be_2O_5$ IC-002491

Beryllium carbonate hydroxide ($Be_2(CO_3)(OH)_2$)

[μ-[Carbonato(2−)-O:O′]]dihydroxydiberyllium, HCI. Basic beryllium carbonate

[54685-97-1]

$Be_2(OH)_2CO_3$ or $Be(OH)_2.BeCO_3$

M 112.0

All references to beryllium carbonate in the early literature prob. refer to basic beryllium carbonate. Formed as reaction between aq. solns. of Be salts and Na_2CO_3 or $NaHCO_3$. Alternatively produced by direct blending of aq. $BeSO_4$ with cryst. $[NH_4]CO_3$. Colourless powder. Dec. on heating to BeO.$BeCO_3$ and then to BeO.

▷ Highly toxic; suspected carcinogen.

Non-basic: [13106-47-3]. *Beryllium carbonate ($BeCO_3$)*

$CBeO_3$ M 69.0

See comment above.

▷ DS2400000.

Gupta, A.K.S., *J. Indian Chem. Soc.*, 1960, **37**, 473 (*synth*)

Gmelin-Podkletnova, V.I. *et al. C.A.*, 1962, **56**, 11426d (*synth*)

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **3**, 474 (*rev, uses*)

Rossi, S.D. *et al. Spectrochim. Acta*, 1964, **20**, 781 (*ir*)

Sinyarev, M.S.R., *J. Therm. Anal.*, 1992, **25**, 355 (*thermal dec*)

CH_2BrCl IC-002492

Bromochloromethane, 9CI, 8CI

Methylene bromochloride. Methylene chlorobromide. Halon 1011. Fluorocarbon 30B1

[74-97-5]

$BrCH_2Cl$

M 129.3

Intermed. for org. synth., fire extinguishant. Liq. with sweet odour, d_4^{25} 1.930. Fp −88°. Bp 67.8°.

▷ Highly toxic and mutagenic, suspected human carcinogen. Irritant, OES 1050 mg m⁻³. PA5250000.

Aldrich Library of FT-IR Spectra, 1st Ed., 1985, **1**, 718 (*ir*)

Aldrich Library of NMR Spectra, 2nd Ed., 1983, **2**, 728 (*pmr*)

Henry, L., *J. Prakt. Chem.*, 1885, **32**, 431 (*synth*)

Stevens, C.L. *et al. J. Am. Chem. Soc.*, 1956, **78**, 2564 (*synth*)

Crews, A.C. *et al. J. Pharm. Pharmacol.*, 1957, **9**, 824 (*synth*)

Lindeman, W.M. *et al. J. Am. Chem. Soc.*, 1960, **90**, 1400 (*rev*)

Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 209

Sax, N.I. *et al. Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 502

CH_2BrF IC-002493

Bromofluoromethane, 9CI

Methylene bromofluoride. Fluorocarbon 31B1

[373-52-4]

CH_2BrF

M 112.9

Liq. Bp 18-20°.

▷ Highly toxic by inhalation.

U.S. Pat., 271 666, (1955); *CA*, **50**, 7845 (*synth*)
Kushina, I.D. *et al*, *CA*, 1974, **80**, 26704 (*synth*)

IC-002494

CH_2BrNO_2

Bromonitromethane, 9CI
Nitromethyl bromide
[563-70-2]

$BrCH_2NO_2$

M 139.9
Liq. Bp_{742} 148-149°, $Bp_{40\text{-}50}$ 70-72°.

Sherrill, M.L., *J. Am. Chem. Soc.*, 1924, **46**, 2753 (*synth*)
Ohishi, Y. *et al*, *Chem. Pharm. Bull.*, 1984, **32**, 4260 (*synth, pmr, ir*)
Fishwick, B.R. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1171 (*synth, pmr, use*)

IC-002495

CH_2Br_2

Dibromomethane, 9CI
Methylene bromide. R 30B2
[74-95-3]

CH_2Br_2

M 173.8
Solvent, reagent for org. synth. Liq. Spar. sol. H_2O. d_{25}^{25} 2.48. Fp −52.7°. Bp 97°.

▷ Mod. toxic. Reacn. with K metal produces shock-sensitive explosive. PA7350000.

Org. Synth., Coll. Vol., 1, 1932, 357 (*synth*)
Kawaguchi, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 57 (*cryst struct*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 273.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1112.

IC-002496

CH_2ClI

Chloroiodomethane
[593-71-5]

$ClCH_2I$

M 176.3
Versatile organic synthon. Commercially available. Liq. Bp 108-109° (104-105°).

Miyano, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 2864 (*synth, pmr*)
Hahn, R.C., *J. Org. Chem.*, 1988, **53**, 1331 (*synth, bibl, use*)

IC-002497

CH_2Cl_2

Dichloromethane, 9CI
Methylene chloride. Methane dichloride. R 30
[75-09-2]

CH_2Cl_2

M 84.9
Manuf. by chlorination of chloromethane. Widely used solv. used in coffee decaffeination. Component of paint removers. Blowing agent in foams. Volatile liq. d_4^{15} 1.335. Fp −96.8°. Bp 40.1°.

▷ Mod. toxic, eye irritant. OES 350 mg m^{-3}. Exp. carcinogen at high dose level. Gives explosive mixts. with various materials. Vapour can ignite or explode if heated. Dec. to toxic $COCl_2$ if strongly heated in air. PA8050000.

Panizzon, L., *Helv. Chim. Acta*, 1932, **15**, 1191 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, 2, 273; **7**, 239.
Kawaguchi, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 62 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 686 (*rev*)
Bretherick, L., *Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 280.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2215.

IC-002498

CH_2Cl_2S

Chloromethylsulfenyl chloride
[26826-80-2]

$ClCH_2SCl$

M 116.9
Synth. from Me_2S_2 + Cl_2 at −20°. Orange liq., slowly dec. in H_2O; stable in dry air. Sol. $CHCl_3$, C_6H_6. Bp_{40} 50°.

Brintzinger, H. *et al*, *Chem. Ber.*, 1950, **83**, 87 (*synth*)

IC-002499

$CH_2Cl_3OPt^{\ominus}$

Carbonyltrichlorodihydroplatinate(*IV*)(1−), 9CI
[42562-39-0]

$[Pt(CO)H_2Cl_3]^{\ominus}$

M 331.4 (ion)
Struct. not determined. May be identical to Carbonyltrichloroplatinate(*II*)(1−), IC-002364. Synth. from $Pt(CO)_2$ + HCl aq. + $Fe^{3\oplus}$.

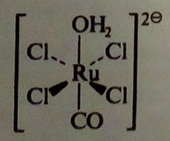
Et_4N salt: [32679-18-8].
Air-stable pale yellow solid. Sol. $CHCl_3$, EtOH, Me_2CO.

Rachovskaya, L.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1972, **17**, 1173 (*synth, ir*)

IC-002500

$CH_2Cl_4O_2Ru^{2\ominus}$

Aquacarbonyltetrachlororuthenate(2−)



M 288.9 (ion)
Prepd. by reducing $RuCl_3.xH_2O$ with boiling HCOOH/aq. HCl. Sol. H_2O, aq. HCl (green soln.). Ir ν_{CO} 1950 cm^{-1} (aq. HCl).

Di-NH_4 salt: [14912-60-8].
Pale-green cryst. Ir ν_{CO} 1950 cm^{-1} (KBr).

Di-Cs salt: [17568-72-8].
Air-stable green solid. Dec. at ca. 250°. Ir ν_{CO} 1951; ν_{RuCl} 311, 289 cm^{-1} (nujol).

[30420-20-3]

Halpern, J. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 5142 (*synth, ir*)
Colton, R. *et al*, *Aust. J. Chem.*, 1967, **22**, 2011; 1971, **24**, 903 (*synth, ir*)
Cleare, M.J. *et al*, *Chem. Ind.* (*London*), 1967, 1705 (*synth*)
Stanko, J.A. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 5580 (*cryst struct*)

IC-002501

CH_2F_2

Difluoromethane, 9CI
Fluorocarbon 32
[75-10-5]

CH_2F_2

M 52.0
Prepd. by reaction of CH_2Cl_2 with HF over chromium catalyst. Low-temp. refrigerant. Gas. Fp −136°. Bp −51.6°.

U.S. Pat., 2 745 886, (1956).
Hasek, W.R. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 543 (*synth*)
Verbeek, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1966, **5**, 314 (*synth*)
Lazzeretti, P. *et al*, *Org. Magn. Reson.*, 1971, **3**, 113 (*nmr*)
Burton, D.J. *et al*, *J. Org. Chem.*, 1975, **40**, 2796 (*synth*)
Mizuno, M. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 1077 (*ir*)

IC-002502

$CH_2F_2N_2O$

***N,N*-Difluorourea, 9CI**
[1510-31-2]

H_2NCONF_2

M 96.0
Synth. from F_2 + $(NH_2)_2CO$ + H_2O. Non-hygroscopic needles (CH_2Cl_2/CCl_4), hygroscopic platelets by subl. Mp 41-41.5°. Oxid. by HI. Dec. at −20° in conc. aq. soln.

▷ Toxic.

Banks, R.E. *et al*, *J. Chem. Soc. C*, 1966, 1514.
Inorg. Synth., 1970, **12**, 307 (*synth, F-19 nmr*)
Grakauskas, V. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 2096 (*synth*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1255 (*haz*)

IC-002503

CH_2F_4S

Tetrafluoromethylenesulfur, 9CI
Methylenesulfur tetrafluoride
[66793-25-7]

$H_2C{=}SF_4$

M 122.0
Gas. Mp −139°. Bp −19°.

Kleemann, G. *et al*, *Chem. Ber.*, 1983, **116**, 645 (*synth, ir, raman, nmr, ms*)

IC-002505

$CH_2F_{10}N_2OS_2$

Decafluoro[μ-(ureato-*N*:*N'*)]disulfur, 9CI
N,N'-*Bis*(*pentafluorothio*)*urea*
[55683-04-0]

$F_5SNHC(O)NHSF_5$

M 312.1
Formed from F_5SNCO + F_5SNH_2 or SF_3N + COF_2. Stable white cryst. Mod. sol. Et_2O, MeOH, Me_2CO, insol. $CHCl_3$, CCl_4. Dec. at 123°.

Duncan, L.C. *et al*, *J. Inorg. Nucl. Chem.*, 1976, 33 (*synth, ir, pmr, F-19 nmr, ms, reactions*)
Thrasher, J.S. *et al*, *J. Fluorine Chem.*, 1984, **24**, 431 (*synth*)

IC-002506

$CH_2F_{10}S_2$

Bis(pentafluorosulfur)methane
Methylenebis(*pentafluorosulfur*)
[117146-25-5]

$F_5SCH_2SF_5$

M 268.1
Formed by hydrol. of $(F_5S)_2C{=}CF_2$. Colourless liq. Bp 67°.

Gerhardt, R. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1988, **27**, 1534 (*synth, pmr, F-19 nmr, ir, ms*)

IC-002507

CH_2I_2

Diiodomethane, 9CI
Methylene iodide
[75-11-6]

CH_2I_2

M 267.8
Liq. Spar. sol. H_2O. d_{15}^{15} 3.33. Mp 6°. Bp 181° part. dec., Bp_{70} 106-107°.

▷ PA8575000.

Org. Synth., Coll. Vol., 1, 1932, 358 (*synth*)
Altabev, N. *et al*, *Chem. Ind.* (*London*), 1973, 331 (*synth*)
Kawaguchi, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 57 (*cryst struct*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 820.

IC-002508

CH_2NO_3P

Cyanophosphonic acid, 9CI

$(HO)_2P(O)CN$

M 107.0
Di-Et ester: [2942-58-7].
$C_5H_{10}NO_3P$ M 163.1
Reagent for amide synth. Oil. Bp_{20} 103-104°.

▷ TD2500000.

Yamada, S. *et al*, *Tetrahedron*, 1976, **32**, 2211 (*synth, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, 7, 107 (*use*)

IC-002509

CH_2N_2

Cyanamide, 11CI
Carbodiimide. Carbamic acid nitrile. Hydrogen cyanamide
[420-04-2]

$H_2NC{\equiv}N$ (C_s)

M 42.0
Behaves chemically as the diimide HN=C=NH. Manuf. from limestone, coke and N_2. Synth. from $CaCN_2$ + H_2O/H_2SO_4. Commercially available. White cryst. (C_6H_6/Et_2O). Sol. H_2O, EtOH, Et_2O, $CHCl_3$, C_6H_6. Mp 46°. Bp_{19} 140°. Steam-volatile; hydrol. by $H^{\oplus}$ or $OH^{\ominus}$ to urea. Converted by dil. $OH^{\ominus}$ into dicyanodiamide. n_D^{48} 1.442.

▷ Mod. toxic, TLV 2. Dec. violently > 50° in contact with H_2O, acids or alkalis. Strong irritant, caustic; produces dermatitis. GS5950000.

Inorg. Synth., 1950, **3**, 39 (*synth*)
Fieser, M. *et al*, *Fieser and Fieser's Reagents for Organic Synthesis*, Wiley, 1967, **1**, 170; 1972, **3**, 71; 1975, **5**, 168 (*use*)
Tyler, J.K. *et al*, *J. Mol. Spectrosc.*, 1972, **43**, 1248 (*struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **7**, 291.
Denner, L. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 1979 (*cryst struct*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 981 (*tox*)

$CH_2N_2S_3$ IC-002510

$1\lambda^4,3\lambda^4,5,2,4$-Trithiadiazine

[114078-94-3]

M 138.2
Stable red cryst. solid. Mp 43-45°.
1-Oxide: [114102-66-8].
$CH_2N_2OS_4$ M 154.2
Cryst. Mp 96-97°.

Bannister, R.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1546 (*synth, ir, pmr, cryst struct*)
Bannister, R.M. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1989, 2503 (*synth, ir, pmr*)
Bannister, R.M. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1990, 509 (*synth, oxide*)

CH_3N_3O IC-002511

Carbamic azide, 9CI

Carbamoyl azide, 8CI

[13125-56-9]

H_2NCON_3

M 86.0
Cryst. Mp 92-93°, Mp 96-98°.

Thiele, J. *et al*, *Justus Liebigs Ann. Chem.*, 1894, **283**, 37 (*synth*)
Hofmmer, R. *et al*, *Z. Elektrochem.*, 1949, **53**, 383 (*synth*)
Heesing, A. *et al*, *Chem. Ber.*, 1970, **103**, 539 (*synth*)

$CH_2Na_2O_4$ IC-002512

Sodium carbonate monohydrate

Carbonic acid, disodium salt monohydrate. Crystal carbonate

[5968-11-6]

$Na_2CO_3.H_2O$

M 124.0
Commercially available. Synth. by thermal dec. of the decahydrate over conc. H_2SO_4. Colourless orthorhombic deliquescent cryst. Dec. on heating by H_2O loss ($-H_2O$ at 100°). V. sol. H_2O; insol. EtOH, Et_2O. ΔH_f° −1433.9 kJ mol^{-1}; ΔG_f° −1291.3 kJ mol^{-1}; S° 170 J K^{-1} mol^{-1}.
▷ Irritant.
Mineral-form [15490-92-3]
Thermonatrite
Deposit from saline lakes and in arid areas. Colourless, grey or yellow cryst.

Harper, J.P., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1936, **95**, 266 (*cryst struct*)
Bauer, T.W. *et al*, *Can. J. Chem.*, 1952, **30**, 76 (*thermochem data*)

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **18**, 458 (*rev, uses*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 309; 1966, **3**, 1328 (*rev, bibl*)
Wu, K.K. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 890 (*nd, cryst struct*)
Groenveld, F. *et al*, *J. Chem. Thermodyn.*, 1983, **15**, 881 (*cryst struct*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3135A (*haz*)

CH_2OS_2 IC-002513

Dithiocarbonic acid

Carbonodithioic acid, 11CI, 9CI

[4741-30-4]

$S{=}C(OH)SH \rightleftharpoons O{=}C(SH)_2$

M 94.1
Acid unknown in free state.
S,S-Di-Me ester: [868-84-8].
$C_3H_6OS_2$ M 122.2
Liq. Bp 168°.
S-Me, S-Et ester: [10596-55-1].
$C_4H_8OS_2$ M 136.2
Liq. Bp_{10} 83-85°.
S,S-Di-Et ester: [623-80-3].
$C_5H_{10}OS_2$ M 150.2
Liq. Bp 196-197°, Bp_{14} 83-86°.

Schmidt, R. *et al*, *Ber.*, 1868, **1**, 166 (*synth*)
Delépine, M., *Bull. Soc. Chim. Fr.*, 1903, **29**, 56 (*synth*)
Holsber, D.H. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1972, **391**, 1371 (*synth*)
Komati, K. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 3807 (*synth*)

CH_2OSe IC-002514

Methaneselenoic acid, 9CI

Selenoformic acid

HC(Se)OH

M 108.9
tert-Butyl ester: [102737-62-2].
$C_5H_{10}OSe$ M 165.0
Cryst. (hexane at −30°). Mp 50.5-51.5°.
Amide: [92609-97-7]. *Methaneselenoamide, 9CI*
CH_3NSe M 108.0
Yellow needles (Et_2O). Mp 35-37°.
Dimethylamide: [31646-15-8]. *N,N-Dimethylmethaneselenoamide*
C_3H_7NSe M 136.0
Mp 2-4°. $Bp_{0.4}$ 79°.

Collard-Charon, C. *et al*, *Bull. Soc. Chim. Belg.*, 1963, **72**, 304 (*synth, ir*)
Henriksen, L., *Synthesis*, 1974, 501 (*ir, pmr, uv*)
Geisler, K. *et al*, *Z. Chem.*, 1984, **24**, 99 (*amide*)
Ishii, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 2529 (*synth, pmr, ms*)

CH_2O_2S IC-002515

Thiocarbonic acid, 8CI

Carbonothioic acid, 9CI

[10016-32-7]

$HOCOSH \rightleftharpoons HOCSOH$

M 78.0
Known only as derivs.
O,S-Di-Me ester: [38103-95-6].
$C_3H_6O_2S$ M 106.1

Oil with ethereal odour. Bp 120-121°.
O-Di-Me ester: [1115-13-5].
$C_3H_6O_2S$ M 106.1
Bp 119-120°.
O,S-Di-Et ester:
$C_5H_{10}O_2S$ M 134.1
Bp 156°.
O-Di-Et ester: [762-03-8].
$C_5H_{10}O_2S$ M 134.1
Bp 158-159°.
O,S-Di-Ph ester:
$C_{13}H_{10}O_2S$ M 230.2
Needles (EtOH). Mp 56°.
O-Di-Ph ester: [13509-34-7].
$C_{13}H_{10}O_2S$ M 230.2
Plates (EtOH). Sol. most org. solvs.; insol. H_2O. Mp 106°.
Anhydride: see *Carbonyl sulfide, IC-002778*
Chloride: see *Carbonothioic dichloride, IC-002354*
Hydrazide: see *Thiocarbohydrazide, IC-002622*
Nitrile: see *Thiocyanic acid, IC-002479*

Delépine, M., *Ann. Chim. (Paris)*, 1912, **25**, 547.
Oki, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 1995 (*conformn*)

CH_2O_3 IC-002516

Carbonic acid

[463-79-6]

$(HO)_2C{=}O$

M 62.0
Present in aq. solns. of CO_2, the hydration of CO_2 being a slow reaction. Forms a wide range of salts $M[HCO_3]$ and M_2CO_3. Represents part of the carbon cycle in aquatic media. pK_{a1} 6.36, pK_{a2} 10.33 (25°). True diss. const. $[H^\oplus][HCO_3^\ominus]/H_2CO_3 \sim 0.00025$.
NH_4 salt (1:1): [1066-33-7]. *Ammonium bicarbonate. Ammonium hydrogen carbonate*
CH_5NO_3 M 79.0
Synth. from aq. NH_3 + CO_2. Commercially available. Used in bakery processes. White solid. Dec. below Mp. to NH_3 + CO_2 + H_2O. V. sol. H_2O.
▷ BO8600000.
Mono-Na salt: see *Sodium hydrogen carbonate, IC-002485*
Mono-K salt: see *Potassium hydrogen carbonate ($KHCO_3$), IC-002471*
Mono-Cs salt: see *Caesium hydrogen carbonate ($CsHCO_3$), IC-002463*
Di-Na salt: see *Sodium carbonate (Na_2CO_3), IC-002771*
Di-Rb salt: see *Rubidium carbonate (Rb_2CO_3), IC-002785*
Di-Cs salt: see *Caesium carbonate (Cs_2CO_3), IC-002385*
Be salt: see *Beryllium carbonate hydroxide ($Be_3(CO)_3(OH)_2$), IC-002491*
Mg salt: see *Magnesium carbonate, IC-002742*
Ca salt: see *Calcium carbonate ($CaCO_3$), IC-002320*
Sr salt: see *Strontium carbonate ($SrCO_3$), IC-002786*
Ba salt: see *Barium carbonate ($BaCO_3$), IC-002284*
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1925, **6**, 72; 1964, **8/1** (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936; *Syst. No.* 14, 1973, **C3**, 36 (*bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 1232 (*rev*)
Palmer, D.A. *et al*, *Chem. Rev.*, 1983, **83**, 651 (*rev*)
Terlouw, J.K. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1990, **29**, 404 (*struct*)

$[CH_2O_6P_2Tc^{4\ominus}]$ IC-002517

Methylenediphosphonate technetium complex

Medronate-Tc. MDP-Tc. Technetium-MDP. Osteolite. Macrotec

[101488-09-9]

$[O_3PCH_2PO_3]^{4\ominus}$ + Tc

Ill-defined methylenediphosphonate (MDP) complexes of technetium(*III*),(*IV*), and (*V*) are prepared by reduction of $TcO_4^\ominus$. They may be oligomeric - their nature and ratio depends on method of preparation. There is a well-defined hydroxo-derivative ($CH_3O_7P_2Tc^\ominus$) and a nitrido-technetium(*VI*) species. Synth. by electrochemical, $S_2O_4^{2\ominus}$, $BH_4^\ominus$, or Sn(*II*) reduction of $TcO_4^\ominus$. Tc(*IV*) species are synth. by reaction of $TcBr_6^{2\ominus}$ with MDP. Amongst the most widely used Tc compds, mainly for bone imaging but also for imaging the spleen, brain, and kidneys, and for labelling red blood cells.

Libson, K. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 2476 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, *Suppl. Vol.* 2, 1983, 212 (*bibl*)
Tanabe, S. *et al*, *Int. J. Appl. Radiat. Isot.*, 1983, **34**, 1577, 1585 (*synth, characterisation, hplc*)
Hoffman, T.J. *et al*, *Int. J. Appl. Radiat. Isot.*, 1984, **35**, 223 (*hplc*)
Pauwels, E.K.J. *et al*, *Nucl. Med. Commun.*, 1984, **5**, 467 (*synth, characterisation*)
Baldas, J. *et al*, *Int. J. Appl. Radiat. Isot.*, 1985, **36**, 133 (*synth*)
Najafi, A. *et al*, *J. Nucl. Med.*, 1985, **26**, 524 (*synth, characterisation, hydrol*)
Handeland, A.M.L. *et al*, *Appl. Radiat. Isot.*, 1987, **38**, 479 (*oxidn state, radiochromatog*)
Martin, J.L. *et al*, *Inorg. Chem.*, 1989, **28**, 2899 (*exafs*)

$[CH_2O_7P_2Tc]$ IC-002518

Technetium (hydroxymethylene)bisphosphonate

(Hydroxymethylene)bisphosphonic acid technetium salt, 11CI. Oxidronic acid technetium salt. HDP-Tc

[72945-61-0]

Struct. unknown

Incomplete formula given. Ill-defined complex prep. by $TcO_4^\ominus$ redn. in presence of ligand. Commercially available bone imaging agent - high bone affinity and fast blood clearance.

Wang, T.S.T. *et al*, *J. Nucl. Med.*, 1980, **21**, 767 (*synth*)
Johnson, J.A. *et al*, *J. Nucl. Med.*, 1988, **29**, 1347 (*pharmacol*)
Weber, D.A. *et al*, *J. Nucl. Med.*, 1989, **30**, 1117 (*pharmacol*)

CH_2S IC-002519

Thioformaldehyde

Methanethial

[865-36-1]

$H_2C{=}S$

M 46.0
Formed by pyrolysis of Me_2S_2 or 1,3,5-Trithiane, IC-003631 with matrix isol., or from MeSH + hν. $t_{\frac{1}{2}}$ approx. 6 min at 0.01 mm.
Dimer: see *1,3-Dithietane, IC-003119*
Trimer: see *1,3,5-Trithiane, IC-003631*
S-oxide: [40100-16-1]. *Thioformaldehyde S-oxide. Methanethiol S-oxide. Sulfine*
CH_2OS M 62.0
Formed by pyrolysis of DMSO and related compds. with matrix isolation. Interatomic distances: H—C 108.5, C—S 161.0, S—O 146.9 pm; angle: CSO 114.7°.

Johns, J.W.C. *et al, J. Mol. Spectrosc.*, 1971, **39**, 479 (*ir*)
Beers, Y. *et al, J. Mol. Spectrosc.*, 1972, **44**, 553 (*microwave*)
Jacox, M.E. *et al, J. Mol. Spectrosc.*, 1975, **58**, 142 (*ir*)
Block, E. *et al, J. Am. Chem. Soc.*, 1976, **98**, 1264 (*oxide, microwave*)
Powers, D.E. *et al, J. Chem. Phys.*, 1979, **83**, 1890 (*oxide, ir, isol*)

IC-002520

CH_2S_2
Methanedithioic acid, 9CI
Dithioformic acid. Dithiomethanoic acid
[4472-10-0]

HCSSH

M 78.1
K salt. Cryst. Mp 196°.
Gattow, G. *et al, Naturwissenschaften*, 1971, **58**, 53; *CA*, **74**, 82598 (*synth*)
Engler, R. *et al, Z. Anorg. Allg. Chem.*, 1976, **31**, 995 (*pmr*)
Bak, B. *et al, J. Mol. Spectrosc.*, 1978, **69**, 401 (*synth*)
Auberg, E. *et al, J. Mol. Struct.*, 1979, **57**, 95 (*struct*)

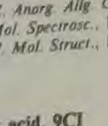
IC-002521

CH_2S_3
Carbonotrithioic acid, 9CI
Trithiocarbonic acid. Carbon sulfide di(hydrogen sulfide)
[594-08-1]

$S{=}C(SH)_2$

M 110.2
Synth. from $BaCS_3$ + HCl at 0°. Liq. Sol. H_2O, CCl_4. d^{25} 1.476. Mp −26.9°. pK_{a1} 2.68, pK_{a2} 8.18. Salts give red aq. solns.
Di-Na salt: Yellow needles (EtOH). Mp 80°.
Di-Me ester: [2314-48-9].
$C_3H_6S_3$ M 138.2
Yellow oil. Bp_{10} 90°.
▷ FG2975000.
Di-Et ester:
$C_5H_{10}S_3$ M 166.3
Yellow oil. Bp_7 130°.
Yeoman, E.W., *J. Chem. Soc.*, 1921, 38 (*salts*)
Gattow, G. *et al, Z. Anorg. Allg. Chem.*, 1963, **321**, 143 (*synth, ir, uv*)
Philippot, E., *Rev. Chim. Minér.*, 1967, **4**, 643 (*salts, rev*)
Tomita, K. *et al, Chem. Pharm. Bull.*, 1972, **20**, 2302 (*deriv*)
Claudio, B. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2419 (*metal complexes*)
Lee, A.W.M. *et al, Synth. Commun.*, 1988, **18**, 1531 (*synth*)
Barbero, M. *et al, Synthesis*, 1988, 22 (*Di-Me ester, synth, pmr, use*)

CH_2S_6 IC-002522
Hexathiepane, 9CI
1,2,3,4,5,6-Hexathiacycloheptane
[17233-71-5]



M 206.4
Minor constit. of *Lentinus edodes*. Mp 90°.
Katsura, M. *et al, Chem. Pharm. Bull.*, 1967, **15**, 988 (*isol, synth*)
Fehér, F. *et al, Z. Naturforsch., B*, 1969, **24**, 1485 (*synth*)
Fehér, F. *et al, CA*, 1976, **85**, 54924c (*cryst struct*)

CH_2Se IC-002523
Selenoformaldehyde
Methaneselenal, 9CI
[6596-50-5]

$H_2C{=}Se$

M 92.9
V. unstable, detected by various spectroscopic techniques. Stabilised as complexes.
▷ LP9800000.
Trimer: see *1,3,5-Triselenane, IC-003632*
Hofmann, L. *et al, J. Organomet. Chem.*, 1983, **255**, C41
Bock, H. *et al, Chem. Ber.*, 1984, **117**, 187 (*pe, theory*)
Judge, R.H. *et al, J. Am. Chem. Soc.*, 1984, **106**, 5406
Glinski, R.J. *et al, J. Am. Chem. Soc.*, 1986, **108**, 531

CH_2Te_2 IC-002524
Methylene ditelluride
[94111-12-3]

$(CH_2Te_2)_n$

M 269.2
Polymeric, probably with chain and/or ring struct. Formed by reduction of $(Cl_3Te)_2CH_2$ in aq. soln. Solid. Insol.
Dirk, C.W. *et al, J. Am. Chem. Soc.*, 1985, **107**, 675 (*synth, reactions, nmr*)
Takashi, N. *et al, J. Chem. Soc., Chem. Commun.*, 1985, 269 (*conductivity*)

CH_3AgO_3S IC-002525
Silver(*I*) methylsulfonate
(*Methanesulfonato*)*silver*(I)

$AgOSO_2Me$

M 202.9
Distorted trigonal bipyramidal coordination about Ag; the methanesulfonato groups act as pentacoordinating ligands. Cryst.
Charbonnier, F. *et al, J. Appl. Crystallogr.*, 1975, **8**, 694 (*synth, powder struct*)
Charbonnier, F. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2824 (*cryst struct*)

CH_3BBr_2 IC-002526
Dibromomethylborane, 10CI, 9CI
Methylboron dibromide. Methyldibromoborane
[17933-16-3]

$MeBBr_2$

M 185.6
Liq., sensitive to air and moisture. Bp 60-62°.
Nöth, H. *et al, J. Org. Chem.*, 1968, **12**, 23 (*pmr*)
Berger, H. *et al, Chem. Ber.*, 1976, **109**, 2266 (*nmr*)
Haubold, W. *et al, Z. Anorg. Allg. Chem.*, 1976, **420**, 251 (*synth*)
Schulze, J. *et al, Chem. Ber.*, 1981, **114**, 495 (*use*)
Meler, A. *et al, Chem. Ber.*, 1981, **114**, 2519 (*use*)

CH_3BCl_2 IC-002527
Dichloromethylborane, 10CI, 9CI, 8CI
Methyldichloroborane. Dichloromethylborine
[7318-78-7]

$MeBCl_2$

M 96.7

Easily condensed gas, sensitive to air and moisture. Bp 11°.
Lengyel, B. *et al, Z. Anorg. Allg. Chem.*, 1963, **322**, 103 (*synth*)
Timms, P. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 1525 (*use*)
Wrackmeyer, B. *et al, Chem. Ber.*, 1976, **109**, 2266 (*nmr*)
Haubold, W. *et al, Z. Anorg. Allg. Chem.*, 1976, **420**, 251 (*synth*)
Barlos, K. *et al, Chem. Ber.*, 1977, **110**, 2774 (*nmr*)
Becher, H. *et al, Spectrochim. Acta, Part A*, 1979, **35**, 59 (*ir*)

IC-002528

CH_3BF_2
Difluoromethylborane, 10CI, 9CI
Methyldifluoroborane
[373-64-8]

$MeBF_2$

M 63.8
Air- and moisture-sensitive gas. V.p. 69.5 mm at −97.4°; 286.9 mm at −78.5°.
Burg, A.B. *et al, J. Am. Chem. Soc.*, 1961, **83**, 2667 (*synth*)
Steele, W.C. *et al, J. Am. Chem. Soc.*, 1962, **84**, 1154 (*ms*)
Barlos, K. *et al, Chem. Ber.*, 1977, **110**, 2774 (*nmr*)
Fussstetter, H. *et al, Chem. Ber.*, 1977, **110**, 3172 (*nmr*)
McKean, D.C. *et al, Spectrochim. Acta, Part A*, 1977, **33**, 951 (*ir, raman*)

IC-002529

CH_3BF_2O
Difluoromethoxyborane, 9CI
Difluoromethoxyborine
[381-59-9]

F_2BOMe

M 79.8
Air- and moisture-sensitive solid. Sol. THF. Mp 41-42°.
Goubeau, J. *et al, Z. Phys. Chem.*, 1959, **20**, 15 (*raman*)
Sternach, B. *et al, J. Am. Chem. Soc.*, 1961, **83**, 3384 (*synth*)
deMoor, J.E. *et al, Ber. Bunsenges. Phys. Chem.*, 1963, 429 (*ir*)
deMoor, J.E. *et al, J. Organomet. Chem.*, 1966, **6**, 235 (*nmr*)
Anosov, V.I. *et al, CA*, 1980, **93**, 221317f (*use*)

IC-002530

$CH_3BF_3^{\ominus}$
Trifluoromethylborate(1 −), 10CI
Methyltrifluoroborate

$[MeBF_3]^{\ominus}$

M 82.8 (ion)
Cu salt: [65139-98-2].
CH_3BCuF_3 M 146.3
Proposed intermed. in BF_3 - catalysed reactions of CuMe.
Maruyama, K. *et al, J. Am. Chem. Soc.*, 1977, **99**, 8068 (*props*)
Yamamoto, Y. *et al, J. Am. Chem. Soc.*, 1978, **100**, 3240; 1980, **102**, 2318 (*props*)

IC-002531

CH_3BI_2
Diiodomethylborane
Methyldiiodoborane
[17933-08-3]

$MeBI_2$

M 279.6
Prepd. from $SnMe_4$ and BI_3. Air-, moisture- and light-sensitive red liq.; stored under N_2 at −10°. Sol. CH_2Cl_2. $Bp_{0.01}$ 50°.
Nöth, H. *et al, J. Organomet. Chem.*, 1968, **11**, 399; 1968, **12**, 23 (*synth, nmr*)
Siebert, W. *et al, Chem. Ber.*, 1973, **106**, 1012 (*use*)
Renk, T. *et al, J. Organomet. Chem.*, 1976, **120**, 1 (*use*)
Haubold, W. *et al, Z. Anorg. Allg. Chem.*, 1978, **446**, 45
Esch, I.I. *et al, J. Organomet. Chem.*, 1979, **171**, 141

IC-002532

$CH_3BN^{\ominus}$
(Cyano-*C*)trihydroborate(1 −), 10CI, 9CI
[33195-00-5]

$[H_3BCN]^{\ominus}$

M 39.8 (ion)
Na salt: [25895-60-7]. *Sodium cyanoborohydride*
CH_3BNNa M 62.8
Commercially available either as solid or in soln. (THF or aq. NaOH). Reducing agent for org. functional groups, particularly for reductive amination of ketones. Cryst. ($MeNO_2$). Sol. THF. Mp >242° dec.
▷ Severe poison, flammable solid.
Berschied, J.R. *et al, Inorg. Chem.*, 1970, **9**, 624 (*ir, nmr, raman*)
Wade, R.C. *et al, Inorg. Chem.*, 1970, **9**, 2166 (*synth, ir, nmr*)
Berschied, J.R. *et al, Inorg. Chem.*, 1972, **11**, 930 (*ir, raman, struct*)
Hall, L.W. *et al, Inorg. Chem.*, 1973, **14**, 580 (*nmr*)
Nair, V. *et al, J. Org. Chem.*, 1978, **43**, 5013 (*use, Na salt*)
Hutchins, R.O. *et al, Org. Prep. Proced. Int.*, 1979, **11**, 201 (*rev, use*)
Yamamoto, Y. *et al, CA*, 1980, **92**, 139884j (*synth, props, rev*)

IC-002533

CH_3BO
Carbonyltrihydroboron, 10CI
Borane carbonyl. Carbon monoxide compd. with borane (1:1), 9CI, 8CI. Borane compd. with carbon monoxide (1:1). Borine carbonyl
[13205-44-2]

$H_3B{-}CO$

M 41.8
Wason, S. *et al, Inorg. Chem.*, 1966, **5**, 161 (*synth*)
Mayer, E., *Monatsh. Chem.*, 1971, **102**, 940 (*synth*)
Finn, P. *et al, J. Am. Chem. Soc.*, 1972, **94**, 1540 (*nmr, props*)
Lloyd, D.R. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 947 (*pe*)
Lambert, L. *et al, J. Mol. Spectrosc.*, 1972, **44**, 578 (*ir*)
Carter, J.C. *et al, Appl. Spectrosc.*, 1974, **28**, 427 (*nmr*)
Pepin, C. *et al, J. Mol. Spectrosc.*, 1976, **59**, 43 (*ir*)

IC-002534

CH_3Br
Bromomethane, 9CI
Methyl bromide. R 40B1
[74-83-9]

H_3CBr

M 94.9
Refrigerating agent, fumigant, industrial solv. for extraction of plant oils. Gas with faint chloroform-like odour. Spar. sol. H_2O. Mp −93.7°. Bp 4.5° (3.6°). Forms a hydrate at 0-5°.
▷ Poisonous vapour. OES 20 mg m^{-3}. Irritant, causes burns. Vapour can ignite or explode if strongly heated. PA4900000.
Egan, C.J. *et al, J. Am. Chem. Soc.*, 1938, **60**, 2097 (*props*)
Gallant, R.W., *Hydrocarbon Process.*, 1968, **47**, 128 (*rev*)
Kawaguchi, T. *et al, Bull. Chem. Soc. Jpn.*, 1973, **46**, 53 (*cryst struct*)
Jung, M.E. *et al, Tetrahedron Lett.*, 1978, 4483 (*synth*)
Bretherick, L., *Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 211
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 569

IC-002535

CH_2BrHgS

Bromo(methylthio)mercury

Bromo(methanethiolato)mercury(II)

[2088-02-0]

HgBr(SMe)

M 327.5

Polymeric with extensive S and Br bridging. Cryst. (Py).

Abel, E.W. *et al*, *J. Organomet. Chem.*, 1966, **5**, 260 (*synth*)
Cano, A.J. *et al*, *Rev. J. Chim.*, 1979, **32**, 311 (*synth, cryst struct*)
Bonavoni, P. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 393 (*ir, raman*)

IC-002536

CH_2BrO

Methyl hypobromite

Hypobromous acid methyl ester, 9CI

[28078-73-1]

MeOBr

M 110.9

Used in Hoffmann rearrangements. Generated *in situ*.

Magnus, E. *et al*, *J. Org. Chem.*, 1958, **23**, 2029 (*use*)
Radlick, P. *et al*, *Synthesis*, 1974, 290 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 466 (*synth, use*)

IC-002537

CH_2BrOSn

Tin(*IV*) bromide methoxide

Bromo(methoxy)tin

[57745-09-2]

Sn(OMe)Br

M 229.6

V. pale yellow powder. Mp 180-185°.

Ewings, P.F.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1717 (*synth, ir, mössbauer*)

IC-002538

CH_2BrO_2S

Bromomethanesulfinic acid, 1ICI

[103227-61-8]

$BrCH_2S(O)OH$

M 159.0

Synth. from bromomethane, sulfonyl bromide and Na_2S + $NaHCO_3$. Unstable even at −10°. Sol. Et_2O, H_2O.

King, J.F. *et al*, *Phosphorus Sulfur*, 1983, **25**, 11 (*synth, nmr, uv*)

IC-002539

CH_2BrO_3S

Bromomethanesulfonic acid

$BrCH_2SO_3H$

M 175.0

Na salt: [34239-78-6].
Cryst. (H_2O). Mp 277-281°.
Chloride: [10099-08-8].
CH_2BrClO_2S M 193.4
Bp_{11} 87-89°.
Bromide: [54730-18-6].
$CH_2Br_2O_2S$ M 237.9
Light-yellow oil. Bp 60-68°.

Truce, W.E. *et al*, *J. Org. Chem.*, 1967, **32**, 990 (*synth, ir, pmr*)
Petrjana, R.B. *et al*, *J. Heterocycl. Chem.*, 1974, **11**, 331 (*synth*)
Block, E. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 4568 (*deriv, synth, pmr, ir*)

IC-002540

CH_3BrS

Methanesulfenyl bromide

Thiohypobromous acid methyl ester. Methyl thiohypobromite

[18681-32-2]

MeSBr

M 127.0

Formed from MeSH + Br_2 at −80° or from Me_2S_2 + Br_2 in CH_2Cl_2. Unstable, not isol. in pure state. Sol. CH_2Cl_2.

Helmkamp, G.K. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 1633 (*synth in soln, conductivity, reactions*)
Nagy-Felsobuki, E. *et al*, *Phosphorus Sulfur*, 1979, **7**, 137 (*synth, pe*)

IC-002541

CH_3BrSe

Methaneselenenyl bromide

Selenohypobromous acid methyl ester. Methyl selenohypobromite

[73501-41-4]

MeSeBr

M 173.8

Formed from Me_2Se_2 + Br_2 in CH_2Cl_2 at −10°. Black-red soln. in CH_2Cl_2.

Denis, J.N. *et al*, *Tetrahedron Lett.*, 1979, **29**, 2697 (*synth, nmr*)

IC-002542

CH_3Br_2Te

Tribromomethyltellurium

Methyltellurium tribromide

[20350-53-2]

$MeTeBr_3$

M 382.3

Obt. as mixt. with Me_2TeBr_2. Formed from $TeBr_4$ + $SnMe_4$. Sol. C_6H_6, toluene.

Schumann, H. *et al*, *J. Organomet. Chem.*, 1982, **232**, 147 (*synth, Te-125 nmr*)

IC-002543

CH_3Cl

Chloromethane, 9CI

Methyl chloride

[74-87-3]

H_3CCl

M 50.4

Manuf. by chlorination of methane or by action of HCl on MeOH. Refrigerant. Methylating reagent used in manuf. of silicones and $PbMe_4$, low-temp. solv., extractant. Gas with ethereal odour. Mod. sol. H_2O. Mp −97.7°. Bp −23.7°.

▷ Toxic by inhalation, OES 105 mg m^{-3}. Extremely flammable, flash p. <0°. Ignites or explodes on contact with BrF_3, BrF_5 and some metals. PA6300000.

Norris, J.F. *et al*, *J. Am. Chem. Soc.*, 1924, **46**, 752 (*synth*)
Downie, I.M., *Chem. Ind. (London)*, 1966, 900 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 674.
Austin, G.T., *Chem. Eng. (N.Y.)*, 1974, **81**, 87 (*rev*)
Miyajima, G. *et al*, *Org. Magn. Reson.*, 1974, **6**, 313 (*cmr*)
Ahlstrom, R.C. *et al*, *Kirk-Othmer Encycl. Chem. Technol.*, 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 677 (*rev*)
DeForest, E.M., *Encycl. Chem. Process. Des.*, 1979, **8**, 214 (*rev*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed. Butterworths, London and Boston, 1979, 302.

Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 346.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 838.

IC-002544

CH_3ClF_2S

Chlorotetrafluoromethylsulfur(*VI*)

Methylsulfur chloride tetrafluoride

[72161-32-1]

$MeSClF_4$

M 138.5

Octahedral around S.

cis-form

Formed from $CH_2{=}SF_4$ + HCl. Colourless liq. Mp 8°. Bp 60°.

Kleeman, G. *et al*, *Chem. Ber.*, 1983, **116**, 645 (*synth, ir, F-19 nmr*)

IC-002545

CH_3ClN_2

Chloroformamidine

Carbamimidic chloride

[6869-14-3]

$H_2NC(=NH)Cl$

M 78.5

Formed by action of H_2O on chlorocarbodiimides, $R_2CClN{=}C{=}NCClR_2$, or from $RSC(NH_2){=}NH_2Cl$ + Cl_2 + H_2O. Mp 43-45°.

B, HCl: [29671-92-9]. *Chloroformamidinium chloride*
$CH_4Cl_2N_2$ M 114.9
Mp 175°. More stable than parent compd.
▷ Reaction with perchloric acid forms v. explosive products.

Johnson, T.B. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 176 (*synth*)
Fetyukhin, V.N., *J. Org. Chem. USSR (Engl. Transl.)*, 1982, **18**, 1822 (*synth, hydrochloride, ir*)
Barker, J. *et al*, *Org. Mass Spectrom.*, 1985, **20**, 619 (*ms*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 829 (*haz*)

IC-002546

CH_3ClNiO

Chloro(methoxy)nickel(*II*), 8CI

Chloro(methoxo)nickel(II)

[25280-56-2]

MeONiCl

M 125.1

Probably has cluster or polymeric struct. with octahedral Ni. Light green solid. Sol. MeOH, Me_2CO. Br, I analogues known, also other alkoxy derivs.

[43732-96-3]

Kruger, A.G. *et al*, *Aust. J. Chem.*, 1970, **23**, 1 (*synth*)

IC-002547

CH_3ClOSn

Tin(*II*) chloride methoxide

Chloro(methoxy)tin

[57745-08-1]

Sn(OMe)Cl

M 185.1

White amorphous powder. Mp 330°.

Ewings, P.F.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1717 (*synth, ir, mössbauer*)

IC-002548

CH_3ClO_2S

Methyl chlorosulfite

Chlorosulfurous acid methyl ester, 9CI. 8CI. Methyl chlorosulfurite

[13165-72-5]

$MeOS(O)Cl$

M 114.5

Formed from $SOCl_2$ and MeOH. Dehydrating agent for alcohols. Colourless liq. Readily hydrol. Bp_{10} 35-38°.

Carre, F. *et al*, *Bull. Soc. Chim. Fr.*, 1953, **53**, 1000 (*synth*)
Berti, G., *J. Am. Chem. Soc.*, 1958, **78**, 1313 (*synth*)
Kobayashi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1966, **39**, 1783 (*synth*)
*Fieser and Fieser's Reagents for Organic Synthesis, 30*69, 1967, **1**, 675 (*use*)
Vijayalth, P. *et al*, *J. Chem. Soc. A*, 1971, 890 (*synth, conformn*)
Hilseng, P.V. *et al*, *J. Mol. Struct.*, 1978, **48**, 85 (*synth, ir, conformn*)
Christie, I.L., *J. Org. Chem.*, 1981, **46**, 3533 (*synth, reactions*)

IC-002549

CH_3ClO_2S

Chloromethanesulfonic acid

[40104-07-2]

$ClCH_2SO_3H$

M 130.5

Na salt: [10352-61-3]
Cryst. (MeOH). Mp 261-262°.
Benzylthiuronium salt: Cryst. (EtOH). Mp 97-98°.
Chloride: [3518-65-8]. *Chloromethanesulfonyl chloride*
$CH_2Cl_2O_2S$ M 148.9
Liq. Bp_{11} 90-91°.
▷ Lacrymator. PB7825000.
Bromide: *Chloromethanesulfonyl bromide*
CH_2BrClO_2S M 193.4
Oil. $Bp_{0.8}$ 50-54°.

Org. Synth., Coll. Vol., 5, 1973, 251 (*deriv, synth*)
Smith, T.L. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 3566 (*synth*)
Silhanek, J. *et al*, *Collect. Czech. Chem. Commun.*, 1977, **42**, 524 (*synth, pmr*)
Block, E. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 4568 (*deriv, synth, ir, pmr, use*)

IC-002550

CH_3ClO_2S

Methyl chlorosulfate

Chlorosulfuric acid methyl ester

[812-01-1]

$MeOSO_2Cl$

M 130.5

Formed from SO_2Cl_2 + MeOH. Colourless liq., readily hydrol. Misc. many org. solvs. d^{20} 1.48. Bp_{16} 55-56°.

Binkley, W.W., *J. Am. Chem. Soc.*, 1938, **60**, 2810 (*synth*)
Cox, C.P., *J. Chem. Eng. Data*, 1983, **28**, 134 (*synth, reactions*)

IC-002551

CH_3ClO_4

Methyl perchlorate

Perchloric acid methyl ester

[17043-56-0]

$MeOClO_3$

M 114.4

Not isol. Formed from $AgClO_4$ + MeI in C_6H_6. Used as a soln. in org. solvs. Sol. hexane, dioxan, C_6H_6.

▷ Highly explosive. Heat-, shock- and friction-sensitive.

Kevill, D.N. *et al, Tetrahedron Lett.*, 1976, **52**, 4811 (*synth, reactions*)
Raynor, P.N.G., *Chem. Ber.*, 1977, **13**, 396 (*haz*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 340 (*use*)
Kevill, D.N. *et al, J. Chem. Soc., Perkin Trans. 2*, 1981, 49 (*synth, reactions*)

IC-002552

CH_3ClSe

Methaneselenenyl chloride
Selenohypochlorous acid methyl ester. Methyl selenohypochlorite
[51384-82-8]

MeSeCl

M 129.4
Synth. from Me_2Se_2 + SO_2Cl_2 in CH_2Cl_2 at 0°. Colourless liq.

Koshutin, V.I. *et al, J. Gen. Chem. USSR (Engl. Transl.)*, 1973, **43**, 2212 (*synth, reactions*)

IC-002553

$CH_3Cl_4ORe^{1\ominus}$

Pentachloro(methoxy)rhenate(*IV*)(2−)

$[ReCl_5(OMe)]^{2\ominus}$

M 394.5 (ion)
Di-Cs salt: [20554-66-9].
Synth. from $ReCl_4(MeCN)_2$, HCl in MeOH and CsCl. Cream-yellow cryst.

Rouschias, G. *et al, J. Chem. Soc. A*, 1968, 489 (*synth, ir, props*)

IC-002554

$CH_3Cl_5OTi^{2\ominus}$

Pentachloromethoxytitanate(*IV*)(2−), 11Cl

$[Ti(OMe)Cl_5]^{2\ominus}$

M 256.1 (ion)
Bis(ethyl acetate-O)Mg salt: [93855-78-8].
$C_9H_{19}Cl_5MgO_4Ti$ M 456.6
Synth. from $TiCl_4$ + $MgCl_2$ + MeOH in EtOAc soln. Olefin polym. catalyst.
Bis(pyridinium) salt: [40583-42-4].
Synth. from Ti(acac)Cl_3 with Py and MeOH in CH_2Cl_2 soln. Yellow solid. Mp 175° dec.

Thompson, D. *et al, Inorg. Chem.*, 1973, **12**, 2190 (*synth, ir, pmr, pyridinium salt*)
Albizzati, E. *et al, Makromol. Chem. Rapid Commun.*, 1984, **5**, 673 (*synth, use, Mg salt*)

IC-002555

$CH_3CuN_3O_8$

Dinitrato(nitromethane)copper(*II*)
Copper(II) *nitrate nitromethane complex (1:1)*

$Cu(NO_3)_2(MeNO_2)$

M 248.5
Each Cu has tetragonal pyramidal coordination with square bases linked diagonally, through bridging nitrato groups. Unidentate nitromethane apical with Cu—O 231 pm, cf. Cu—O (nitrate) 195 pm. Blue-green cryst. $(MeNO_2)$.

Logan, N. *et al, Spectrochim. Acta*, 1965, **21**, 857 (*ir*)
Duffin, B. *et al, Acta Crystallogr.*, 1966, **20**, 210 (*synth, cryst struct*)

CH_3F

Fluoromethane, 9Cl IC-002556
Methyl fluoride. Fluorocarbon 41
[593-53-3]

H_3CF

M 34.0
Gas. Mod. sol. H_2O; sol. EtOH, Et_2O. Mp −141.8°. Bp −78.2°. Crit. point 44.9°/58 atm.
▷ Flammable, narcotic in high concentrations. PA9154000.

Cawood, W. *et al, J. Chem. Soc.*, 1932, 2180 (*synth*)
Swarts, F., *Bull. Soc. Chim. Belg.*, 1937, **46**, 10 (*synth*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1750.

CH_3FO_2S

Methanesulfonyl fluoride, 9Cl, 8Cl IC-002557
Mesyl fluoride

$MeSO_2F$

M 98.0
Interatomic distances: S—O 141, S—F 156.1, C—S 175.9 pm. Synth. from $MeSO_2OH$ + HF. Synthetic intermed., commercially available. Colourless liq. d_4^{20} 1.35. Bp 123.124°, Bp_{40} 80°, Bp_{25} 35°.
▷ Corrosive.

Ham, N.S. *et al, Aust. J. Chem.*, 1953, **6**, 33 (*synth, ir, bibl*)
Gramstad, T. *et al, J. Chem. Soc.*, 1956, 173 (*synth, ir*)
Hargittai, I. *et al, J. Mol. Struct.*, 1973, **15**, 399 (*ed*)
Robinson, E.A. *et al, Spectrochim. Acta, Part A*, 1978, **34**, 1249 (*ir, raman*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2216 (*haz*)

CH_3FO_3S

Methyl fluorosulfate IC-002558
Methyl fluorosulfonate. Fluorosulfuric acid methyl ester. Methyl fluorsulfonate. Magic methyl
[421-20-5]

$MeOS(O)_2F$

M 114.0
Synth. from FSO_3H + CH_2N_2 in SO_2ClF at 85° or from FSO_3H + $(MeO)_2SO_2$. Commercially available methylating agent. Good solvent. Volatile colourless liq. Rapidly hydrol. Ethereal odour. Sol. most org. solvs. d 1.41. Mp −95°. Bp 92-94°. n_D^{20} 1.3326.
▷ Extremely toxic to humans. Exposure can be fatal. Skin, eye and mucous membrane irritant. Reacts with H_2O, steam or acid to give corrosive and toxic fumes. LP0720000.

Meyer, J. *et al, Z. Anorg. Allg. Chem.*, 1932, **206**, 24 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1972, **3**, 202; 1974, **4**, 339; 1975, **5**, 445; 1977, **6**, 381; 1979, **7**, 240; 1980, **8**, 340; 1981, **9**, 307.
Alder, R.G., *Chem. Ind. (London)*, 1973, 983 (*use, F-19 nmr, pmr*)
Pletcher, D. *et al, Chem. Ind. (London)*, 1976, 371 (*synth*)
McGarrity, J.F. *et al, J. Am. Chem. Soc.*, 1983, **105**, 3961 (*synth, pmr, cmr*)
Merck Index, 11th Ed., 1989, 5993 (*props, haz*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2316 (*haz*)

$CH_3F_2IO_2$

Difluoromethoxyoxoiodine, 11Cl IC-002559
[89706-06-9]

$MeOI(O)F_2$

M 211.9
Formed from IF_5 + $(MeO)_4Si$ in SO_2. Colourless cryst. Mp 52-53° dec.

Frohn, H.J. *et al, J. Fluorine Chem.*, 1984, **24**, 219 (*synth, F-19 nmr*)

IC-002560

$CH_3F_2S^{\oplus}$

Difluoro(methyl)sulfonium

$[MeSF_2]^{\oplus}$

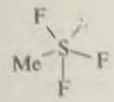
M 85.0 (ion)
Trigonal pyramidal struct. with C_s symmetry. Synth. from $MeSF_3$ + Lewis Acid.
Tetrafluoroborate:
CH_3BF_6S M 171.9
Synth. from $MeSF_3$ + BF_3 in e.g. $CHCl_3$. White solid. Stable under rigorously dry conditions. Sol. HF.
Hexafluoroarsenate:
CH_3AsF_6S M 274.0
Synth. from $MeSF_3$ + AsF_5 in e.g. $CHCl_3$. White solid. Stable under rigorously dry conditions. Sol. HF.

Downs, A.J. *et al, J. Chem. Soc., Dalton Trans.*, 1991, 81 (*synth, ir, raman, pmr, F-19 nmr*)

IC-002561

CH_3F_3S

Methylsulfur trifluoride
Trifluoro(methyl)sulfur
[65082-47-5]



M 104.0
C_s symmetry. Synth. from MeSCl and AgF_2. Unstable at r.t.; can be stored in PTFE at 77K. Reacts with glass, H_2O and air. Sol. CCl_3F (10 g per 100 cm^3 at −23°). Mp −78° → −74°. Bp 80-100°.

BF_3 complex: see *Difluoro(methyl)sulfonium, IC-002560*
Downs, A.J. *et al, Inorg. Chem.*, 1989, **28**, 3286 (*ed*)
Downs, A.J. *et al, J. Chem. Soc., Dalton Trans.*, 1991, 81 (*synth, nmr, ir, raman, reactions*)

IC-002562

CH_3F_3SSi

Silyl trifluoromethyl sulfide
[(*Trifluoromethyl*)*thio*]*silane, 9Cl*
[753-94-6]

H_3SiSCF_3

M 132.1
Synth. from SiH_3I + $Hg(SCF_3)_2$. Gas or liq. Stable when pure at r.t. but dec. in the presence of impurity. Mp −127°. Bp 13.6°.

Downs, A.J. *et al, J. Chem. Soc.*, 1960, 3516 (*synth, ir, nmr*)
Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1978, **447**, 119 (*synth, ir, ms, Si-29 nmr*)

IC-002563

CH_3F_3SeSi

Silyl trifluoromethyl selenide
[(*Trifluoromethyl*)*seleno*]*silane, 9Cl*
[753-96-8]

$H_3SiSeCF_3$

M 179.0
Synth. from SiH_3I + $Hg(SeCF_3)_2$. Liq. Mp −125.8° Bp 35°.

Ebsworth, E.A.V. *et al, J. Chem. Soc.*, 1962, 2290 (*synth, ir, pmr*)
Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1978, **447**, 119 (*synth, ir, ms, Si-29 nmr*)

IC-002564

CH_3F_4IO

Tetrafluoromethoxyiodine
Iodine tetrafluoride methoxide
[38590-00-0]

$MeOIF_4$

M 233.9
Synth. from IF_5 + $(MeO)_4Si$ in SO_2. White solid, readily hydrol. Sol. SO_2, MeCN. Mp 33-34°. Dec. at 80°

Frohn, H.J. *et al, J. Fluorine Chem.*, 1984, **24**, 219 (*synth, F-19 nmr*)

IC-002565

CH_3F_5S

Pentafluoromethylsulfur(*VI*)
[753-79-7]

$MeSF_5$

M 142.0
Formed from $CH_2{=}SF_4$ + HF at −78°. Colourless low-boiling liq., v. inert to LiR or conc. $OH^{\ominus}$. Attacked by Lewis acids. Bp 26°

Kleemann, G. *et al, Angew. Chem., Int. Ed. Engl.*, 1981, **20**, 1037 (*synth, pmr, F-19 nmr*)

IC-002566

$CH_3F_6NOS_2$

Pentafluoro(methylamidosulfurous fluoridato-*N*)sulfur, 10Cl
[84161-13-7]

$FS(OMe){=}NSF_5$

M 223.1
Synth. from $F_3SN{=}SF_2$ + NaOMe. Colourless liq., stable to disproportionation. Vp < 1 mm/25°.

Thrasher, J.S. *et al, J. Fluorine Chem.*, 1981, **18**, 537 (*synth, ms, pmr, F-19 nmr*)

IC-002567

CH_3FeO_2

Iron(*III*) methoxide oxide (Fe(OMe)O)
Methoxyoxoiron(III)
[59473-94-8]

FeO(OMe)

M 102.8
Layer structure; layer spacing 997 pm. Brown solid. Insol. MeOH. Ir ν_{CO} 1050 cm^{-1}.

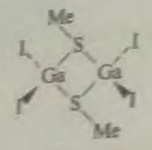
Kikkawa, S. *et al, Inorg. Chem.*, 1976, **15**, 2195 (*synth, mössbauer, struct*)
Son, S. *et al, Inorg. Chem.*, 1980, **19**, 262 (*synth, ir, thermal anal*)
Inorg. Synth., 1983, **22**, 87 (*synth*)

Choy, J.H. et al, Bull. Korean Chem. Soc., 1985, **6**, 251 (*synth, ir*)
Villieras, J. et al, Rev. Chim. Miner., 1985, **22**, 209; *CA*, **103**, 188344n (*synth, mössbauer, cryst struct*)

IC-002568

CH_3GaI_2S

Diiodo(methanethiolato)gallium
Diiodo(methylthio)gallane
[88189-09-7]



dimer

M 370.6
Dimeric.
Dimer: [97092-80-3]. *Tetraiodobis[μ-(methanethiolato)] digallium(III), 11CI*
$C_2H_6Ga_2I_4S_2$ M 741.2
Colourless cryst. (CS_2). V. sol. CS_2, Me_2S_2. Heating in Me_2S_2 gives Tetraiodotetrakis[μ-(methanethiolato)]di-μ-thioxotetragallium, IC-004251.

Hoffmann, G.G., Z. Naturforsch., B, 1984, **39**, 352 (*synth, pmr, ir*)
Beardman, A. et al, Inorg. Chim. Acta, 1985, **99**, L39 (*synth, cryst struct*)

IC-002569

CH_3GeNS

Isothiocyanatogermane, 9CI
Germyl isothiocyanate
[16475-45-9]

H_3GeNCS

M 133.7
Synth. from GeH_3Br + AgSCN. Mp 18.6°.

Srivastava, T.N. et al, Can. J. Chem., 1962, **40**, 739 (*synth*)
Davidson, G. et al, Spectrochim. Acta, Part A, 1967, **23**, 2383 (*ir, raman*)
Sullivan, J. et al, J. Mol. Struct., 1980, **60**, 37 (*microwave, ir, raman, struct*)

IC-002570

CH_3IO

Iodosomethane, 11CI
[97551-34-3]

MeIO

M 157.9
Formed from MeI + O_3 + hν in an Ar matrix at 77K.

Hawkins, M. et al, Inorg. Chem., 1985, **24**, 3285 (*synth, ir*)

IC-002571

CH_3IOSn

Tin(*II*) iodide methoxide
Iodo(methoxy)tin
[57745-10-5]

Sn(OMe)I

M 276.6
Orange needles. Mp 150°.

Ewings, P.F.R. et al, J. Chem. Soc., Dalton Trans., 1975, 1717 (*synth, ir, mössbauer*)

CH_3IO_2

Methyl peroxyhypoiodite IC-002572
Peroxyhypoiodous acid methyl ester
[82803-66-5]

MeOOI

M 173.9
Formed in the oxidation/combustion of MeI at 350-500° (MeO_2 + MeI → MeOOI + Me). Not isol.; forms part of a radical chain process.

Antonik, S., Bull. Soc. Chim. Fr., 1982, 128 (*kinetics*)

CH_3IO_3S

Iodomethanesulfonic acid, 9CI IC-002573
[143-47-5]

ICH_2SO_3H

M 222.0
Free acid little studied and apparently not deuct.
Na salt: [126-31-8]. *Methiodal sodium, BAN, INN, ULAN*
Skiodan sodium. Other proprietary names
Radioopaque medium (urographic). Cryst. Sol. H_2O, spar. sol. org. solvs.
▷ PB2250000.
Bromide: [91586-90-2].
CH_2BrIO_3S M 284.9
Pale-violet liq. $Bp_{0.06}$ 78-80°.

Ger. Pat., 532 766, (1929); *CA*, **26**, 480 (*synth*)
Lauer, W.M. et al, J. Am. Chem. Soc., 1935, **57**, 2361 (*synth*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 1577.
Block, E. et al, J. Am. Chem. Soc., 1986, **108**, 4568 (*bromide*)
Negwer, M., Organic-Chemical Drugs and their Synonyms, 6th Ed., Akademie-Verlag, Berlin, 1987, 13.

CH_3IS

Methanesulfenyl iodide, 11CI IC-002574
Thiohypoiodous acid methyl ester. Methyl thiohypoiodite
[86381-89-7]

MeSI

M 174.0
Formed from MeSH + I_2 in gas phase. Not isol. but believed to be thermodynamically stable.

Shum, L.G.S. et al, Int. J. Chem. Kinet., 1983, **15**, 433 (*kinetics, props*)

CH_3KO

Potassium methoxide IC-002575
Methanol, potassium salt, 8CI. Methoxypotassium
[865-33-8]

KOMe

M 70.1
Synth. by dissoln. of K in MeOH. Manuf. by reaction of CaO, ROH (R = C_{1-4} alkyl) and anhydrous KOH. Commercially available. Widely used as a polym. catalyst; base in org. chem. Moisture-sensitive colourless tetragonal cryst. Reacts with H_2O to form MeOH and KOH.
▷ Flammable, corrosive.

Brady, O.L. et al, J. Chem. Soc., 1950, 767 (*uses*)
Weiss, E., Helv. Chim. Acta, 1963, **46**, 2051 (*cryst struct*)
Simonov, A.P. et al, Zh. Prikl. Spektroscopii, Akad. Nauk. Belorussk. SSR, 1965, **3**, 531; *CA*, **64**, 14061c (*ir*)

Ger. Pat., 2 913 579, (1980); *CA*, **93**, 238825 (*manuf*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2966A (*toxic*)

CH_3LiO

Lithium methoxide IC-002576
Methanol, lithium salt, 8CI
[865-34-9]

LiOMe

M 37.9
Commercially available. Prepared by dissolution of Li in anhydrous MeOH. Moisture sensitive white solid; reacts with water to form LiOH and MeOH. Sol. alcohols.
▷ Flammable.

Kecki, Z. et al, Pol. J. Chem. (Rocz. Chem.), 1963, **37**, 881; *CA*, 1964, **60**, 7592b (*raman, pmr*)
Simmons, A.P. et al, Opt. Spektrosk., 1964, **17**, 848; *CA*, 1965, **62**, 11303b (*ir, struct*)
Conrad, W. et al, J. Org. Chem., 1965, **30**, 3498 (*props*)

CH_5N

Methanimine IC-002577
Formamine. Methyleneamine
[2053-29-4]

$H_2C{=}NH$

M 29.0
Interatomic distances: C—H 109.2, C—N 127.3, N—H 102.1 pm; angles: HNC 110.4°, *cis*-HCN 125.1°.
Interstellar molecule; formed by pyrolysis or photolysis of MeN_3, CH_2N_2, $MeNH_2$. $t_{\frac{1}{2}}$ ~ 10 min. at 5 mm.

Milligan, D.E., J. Chem. Phys., 1961, **35**, 1491 (*ir*)
Jacox, M.E. et al, J. Mol. Spectrosc., 1975, **56**, 333 (*ir*)
Pearson, R. et al, J. Chem. Phys., 1977, **66**, 4149 (*microwave*)
Hamada, Y. et al, J. Mol. Spectrosc., 1984, **105**, 70 (*synth, ir*)
Bock, H. et al, Chem. Ber., 1987, **120**, 1961 (*synth, pe, bibl*)

CH_3NOS

Thiocarbamic acid IC-002578
Aminothioformic acid. Carbamothioic acid
[19045-66-0]

$H_2NCOSH \rightleftharpoons H_2NCSOH$

M 77.1
Free acid unknown. Forms two series of esters.
NH_4 salt: [16687-42-6].
Cryst. V. sol. H_2O; spar. sol. EtOH; insol. Et_2O.
S-Me ester: [21325-07-5].
C_2H_5NOS M 91.1
Prisms (Et_2O). Mp 107-108°.
S-Me ester, N-Ac: [34277-65-1].
$C_4H_7NO_2S$ M 133.1
Needles (C_6H_6). Mp 145.5-146°.
S-Et ester: [637-98-9]. *S-Ethyl carbamothioate, 9CI. S-Ethyl thiocarbamate, 8CI. S-Ethyl aminothioformate. Thiourethane*
C_3H_7NOS M 105.1
Has contraceptive props. Plates (C_6H_6). Sol. hot H_2O. Mp 108-109°. The name Thiourethane is applied to both the *S*-Et and *O*-Et (see below) esters.
S-Et ester, N-Ac: [57964-27-9]. *S-Ethyl acetylcarbamothioate, 9CI*
$C_5H_9NO_2S$ M 147.1
Prisms (C_6H_6). Mp 98°.
S-Ph ester: [61642-86-2].
C_8H_9NOS M 167.2
Plates (C_6H_6). Mp 129°.
O-Me ester: [883-43-6].
C_2H_5NOS M 91.1
Mp 43°.
O-Me ester, N-Ac
$C_4H_7NO_2S$ M 133.1
Cryst. (pet. ether). Mp 79-80°.
O-Et ester: [625-57-8]. *O-Ethyl carbamothioate, 9CI. O-Ethyl thiocarbamate, 8CI. O-Ethyl aminothioformate. Xanthogenamide. Thiourethane*
C_3H_7NOS M 105.1
Fungicide. Volatile monoclinic cryst. Spar. sol. H_2O. Mp 40-41° (16°). Dec. on dist.
O-Et ester, N-Ac: [23406-25-7]. *O-Ethyl acetylcarbamothioate, 9CI. O-Ethyl acetylthiocarbamate, 8CI*
$C_5H_9NO_2S$ M 147.1
Prisms (H_2O). Mp 99.5-101°.
O-Et ester, N,N-Di-Me: [17996-36-2]. *O-Ethyl dimethylcarbamothioate, 9CI*
$C_5H_{11}NOS$ M 133.2
Liq. with peculiar odour. d_4^{25} 1.020. Fp 15°. Bp 216°, Bp_{15} 89-89°.
O-Ph ester: [824-48-4].
C_8H_9NOS M 167.2
Needles (EtOH). Mp 132-132.5°.
N-Ph: see Phenylthiocarbamic acid, IC-003718
N-Ph, S-Ph ester: [4910-32-1].
$C_{13}H_{11}NOS$ M 229.3
Mp 125.5-126°.

Weijlard, J. et al, J. Am. Chem. Soc., 1951, **73**, 1487.
Rennschneider, R. et al, J. Am. Chem. Soc., 1951, **73**, 3965.
Rennschneider, R. et al, Monatsh. Chem., 1953, **84**, 1238.
U.S. Pat., 2 602 813, (1953); *CA*, **47**, 7539.
Stenkamp, L., CA, 1954, **48**, 11347.
U.K. Pat., 688 726, (1954); *CA*, **48**, 2091.
U.K. Pat., 811 861, (1959); *CA*, **53**, 20670e (*synth, props*)
Zil'bermans, E.N. et al, Zh. Obshch. Khim., 1963, **33**, 1023.
Walter, W. et al, Angew. Chem., Int. Ed. Engl., 1967, **6**, 281 (*reviews*)
U.S. Pat., 4 066 681, (1975); *CA*, **88**, 136154.
Goerdeler, J. et al, Chem. Ber., 1982, **115**, 2252 (*synth, ester*)
Jorgensen, K.A. et al, Tetrahedron, 1982, **38**, 1163 (*synth, ester*)

CH_5NOSi

Isocyanatosilane, 9CI IC-002579
Silyl isocyanate. (Cyanato-N)silane
[13780-13-7]

H_3SiNCO

M 73.1
Synth. from AgNCO + SiH_3I, or from $(H_3Si)_3N$ + cyanic acid. Liq. Unstable at r.t. in the presence of impurities. Mp −88.6°. Bp 18.1°.

Ebsworth, E.A.V. et al, J. Chem. Soc., 1962, 4844 (*synth, props*)
Ebsworth, E.A.V. et al, J. Chem. Soc. A, 1967, 69 (*synth*)
Glidewell, C. et al, Chem. Phys. Lett., 1972, **16**, 526 (*struct*)
Duckett, J.A. et al, J. Mol. Spectrosc., 1976, **62**, 34; 1981, **86**, 374 (*microwave*)
Barrow, M.J. et al, J. Chem. Soc., Dalton Trans., 1980, 1838 (*cryst struct*)
Arnold, D.E.J. et al, J. Chem. Soc., Dalton Trans., 1981, 1349 (*pmr*)

CH_3NO_2 IC-002580

Carbamic acid

Aminoformic acid

H_2NCOOH

M 61.0

Free acid not known.

▷ Propyl and butyl esters are carcinogenic.

Me ester. [598-55-0]. *Methyl carbamate. Urethylan*

$C_2H_5NO_2$ M 75.0

Mp 54°. Bp 177°, Bp_{14} 82°

▷ FC2450000.

N-Di-Me, Me ester. Methyl dimethylcarbamate. Methyl dimethylaminoformate

$C_4H_9NO_2$ M 103.1

Misc. H_2O. Bp 131°

Ph ester:

$C_7H_7NO_2$ M 137.1

Mp 141°.

Benzyl ester:

$C_9H_9NO_2$ M 151.1

Leaflets. Mp 86°.

Chloride: [463-72-9]. *Carbamic chloride, 9CI. Carbamoyl chloride. Urea chloride (obsol.)*

CH_2ClNO M 79.4

Synth. from phosgene + NH_3. Colourless liq. stable at −80° dec. readily to HCl + HNCO. Mp ~0°. Bp 61-62° dec.

▷ Evolves HCl on standing.

Fluoride: Carbamoyl fluoride. Carbamic fluoride

CH_2FNO M 63.0

Synth. from HNCO + HF in Et_2O. Colourless needles. Slowly hydrol. to HF + HCNO. Sol. Et_2O, H_2O. Mp 47°. Dec. at 60-70° Subl.

Amide: see *Urea, IC-002597*

Azide: see *Carbamic azide, IC-002511*

NH_4 salt: see *Ammonium carbamate, IC-002619*

N-Di-Me, chloride: Chloroformic dimethylamide

C_3H_6ClNO M 107.5

Mp −33°. Bp 167°.

Gattermann, L., *Justus Liebigs Ann. Chem.*, 1888, **244**, 30.
Thiele, J. *et al, Justus Liebigs Ann. Chem.*, 1898, **302**, 249.
Loev, B. *et al, J. Org. Chem.*, 1963, **28**, 3421.
Sepehrnia, B. *et al, Acta Crystallogr., Sect. C*, 1987, **43**, 249 (*cryst struct, ester*)
Ishii, S. *et al, Bull. Chem. Soc. Jpn.*, 1989, **62**, 455 (*synth, esters*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 696.

CH_3NO_2 IC-002581

Carbonimidic acid, 9CI

Imidocarbonic acid, 8CI

[6703-56-6]

$HN{=}C(OH)_2$

M 61.0

Free acid (unknown) is a tautomer of Carbamic acid, IC-002580.

Di-Ph ester: [4513-71-7]. *Diphenyl imidocarbonate*

$C_{13}H_{11}NO_2$ M 213.2

Cryst. (pet. ether). Mp 55°.

Houben, J. *et al, Ber.*, 1913, **46**, 2447 (*synth*)
Hedayatullah, M., *Bull. Soc. Chim. Fr.*, 1967, 416 (*synth*)
Kupfer, R. *et al, Chem. Ber.*, 1986, **119**, 3236 (*synth, ir, pmr, cmr*)

CH_3NO_3Zn IC-002582

Ammine[carbonato(2−)-*O*]zinc

Zinc carbonate ammine complex

[99544-82-8]

$Zn(OCO_2)(NH_3)$

M 142.4

Tetrahedral zinc in chain struct. Exhibits non-linear optical effect. White cryst. Insol. H_2O.

Besançon, P. *et al, Mater. Res. Bull.*, 1985, **20**, 1063 (*synth, cryst struct*)

CH_3NSSi IC-002583

Isothiocyanatosilane, 9CI

Silyl isothiocyanate. (Thiocyanato-N)silane

[14311-54-7]

H_3SiNCS

M 89.1

Synth. from AgNCS + SiH_3I; from $(H_3Si)_3N$ + H_2S + $Hg(NCS)_2$, or from $(H_3Si)_2S$ + AgNCS. Pungent liq. Slowly dec. in air. Rapidly hydrol. by cold H_2O. Mp −51.8°.

MacDiarmid, A.G. *et al, J. Inorg. Nucl. Chem.*, 1955, **1**, 411; 1956, **2**, 88 (*synth, struct*)
Ebsworth, E.A.V. *et al, Trans. Faraday Soc.*, 1962, **58**, 1069 (*ir, raman*)
Ebsworth, E.A.V. *et al, J. Chem. Soc. A*, 1967, 69 (*synth*)
Glidewell, C., *J. Inorg. Nucl. Chem.*, 1969, **31**, 1303 (*synth*)
Glidewell, C. *et al, Chem. Phys. Lett.*, 1972, **16**, 526 (*struct*)
Doessel, K.F. *et al, Z. Naturforsch., A*, 1977, **32**, 462, 473; 1979, **34**, 482 (*microwave*)
Arnold, D.E.J. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1349 (*nmr*)

CH_3NS_2 IC-002584

Dithiocarbamic acid, 8CI

Carbamodithioic acid, 9CI. Aminodithioformic acid. Dithiocarbonic amide

[594-07-0]

H_2NCSSH

M 93.1

Needles, unstable above 20°→ CS_2 + H_2S + NH_4SCN. Sol. EtOH, Et_2O. Mp 35.7°. Dec. by H_2O.

Me ester: [16696-83-6].

$C_2H_5NS_2$ M 107.2

Insol. H_2O. Mp 42°.

Me ester, N-Ac: [16696-88-1].

$C_4H_7NOS_2$ M 149.2

Yellow prisms. Mp 119°.

Et ester: see *Ethyl dithiocarbamate, IC-003637*

NH_4 salt: Ammonium dithiocarbamate

$CH_6N_2S_2$ M 110.2

Synth. from CS_2 and NH_3. Lustrous yellow cryst. Sol. H_2O. Mp 99° dec. Dec. in air.

Mulder, E., *Justus Liebigs Ann. Chem.*, 1873, **168**, 232 (*synth*)
U.K. Pat., 307 728, (1927); *CA*, **24**, 129 (*synth*)
Inorg. Synth., 1950, **3**, 48 (*deriv, synth*)
Org. Synth., Coll. Vol., 3, 1955, 763 (*synth*)
Capacchi, L. *et al, J. Chem. Soc., Chem. Commun.*, 1966, 441 (*deriv, cryst struct*)
Gattow, G. *et al, Z. Anorg. Allg. Chem.*, 1969, **364**, 161 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst.No. 14, 1978, **D6**, 133 (*bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 744.
Merck Index, 11th Ed., 1989, 533 (*deriv, props*)

CH_3NSeSi IC-002585

Isoselenocyanatosilane, 9CI

Silyl isoselenocyanate. (Selenocyanato-N)silane

[16966-41-9]

$H_3SiNCSe$

M 136.0

Synth. from silver selenocyanate + SiH_3I. Liq., polym. slowly at r.t. Mp −15.1°. Bp 111°, Bp_9 20°.

Ebsworth, E.A.V. *et al, J. Chem. Soc.*, 1963, 3893.
Cradock, S. *et al, J. Chem. Soc., Faraday Trans. 2*, 1980, **76**, 860.
1981, **77**, 1257 (*ir*)
Arnold, D.E.J. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1349 (*nmr*)

CH_3NSi IC-002586

Cyanosilane

Silyl cyanide. Silanecarbonitrile, 9CI

[1111-70-2]

H_3SiCN

M 57.1

Referred to as Isocyanosilane in some old literature but has been shown to have the cyanide struct. Synth. by the action of SiH_3I vapour on NaCN or AgNC. Cryst. Rapidly hydrol. by cold H_2O. Mp 32.4°.

Emeleus, H.J. *et al, J. Chem. Soc.*, 1941, 353 (*synth*)
MacDiarmid, A.G., *J. Inorg. Nucl. Chem.*, 1956, **2**, 88 (*synth*)
Linton, H.R. *et al, Spectrochim. Acta*, 1958, **10**, 299 (*ir*)
Sheridan, J. *et al, Proc. Chem. Soc., London*, 1960, 21 (*microwave*)
Arnold, D.E.J. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1349 (*nmr*)
Blair, P.D. *et al, J. Mol. Struct.*, 1989, **193**, 279 (*struct*)

$CH_3N_3O_2S$ IC-002587

Methanesulfonyl azide, 9CI

Mesyl azide

[1516-70-7]

$MeSO_2N_3$

M 121.1

Diazo transfer reagent. d_{20} 1.40. $Bp_{0.5}$ 56°. Unstable above 100°.

▷ Potentially explosive.

Boyer, J.H. *et al, J. Org. Chem.*, 1958, **23**, 1051 (*synth, ir*)
Taber, D.F. *et al, J. Org. Chem.*, 1986, **51**, 4077 (*use*)

CH_3NaO IC-002588

Sodium methoxide

Methanol, sodium salt, 8CI. Methoxysodium. Sodium methylate

[124-41-4]

NaOMe

M 54.0

Synth. by reaction of Na or Na/Hg with dry MeOH in an inert atm. Commercially available as solid or in MeOH soln. Polym. and cyclocondensation catalyst. Powerful nucleophile widely used in org. chem. Moisture-sensitive, white tetragonal cryst. Sol. MeOH. Mp >300°. Reacts with H_2O forming MeOH and aq. NaOH.

▷ Flammable solid; corrosive. PC3570000.

Seubold, F.H., *J. Org. Chem.*, 1956, **21**, 156 (*ir*)
Weiss, E., *Z. Anorg. Allg. Chem.*, 1964, **332**, 197 (*struct*)
Iwakura, Y. *et al, J. Polym. Sci., Part A*, 1967, **5**, 675 (*uses*)
Dubuisc, M. *et al, Bull. Union Physiciens*, 1979, **74**, 351; *CA*, 1980, **92**, 180590 (*uses*)
Pascal, Y.L. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1981, **78**, 675 (*pmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3146D, 3147A (*haz*)

CH_3NaS IC-002589

Sodium thiomethoxide

(Methylmercapto)sodium. Methanethiol, sodium salt, 8CI. (Methylthio)sodium

[5188-07-8]

NaSMe

M 70.0

Synth. by reaction of MeSH with Na in liq. NH_3. Commercially available. Thiolation reagent widely used in org. chem. Tetragonal cryst. Sol. hexamethylphosphoramide. Moisture sensitive. Reacts with H_2O to form MeSH and NaOH.

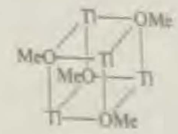
▷ Flammable solid, corrosive.

Weiss, E. *et al, Chem. Ber.*, 1972, **105**, 481 (*synth, struct*)
Hartke, K. *et al, Arch. Pharm.*, 1980, **313**, 1029 (*uses*)
Testaferri, L. *et al, Tetrahedron Lett.*, 1980, **21**, 3099 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3157A (*haz*)

CH_3OTl IC-002590

Thallium(*I*) methoxide

[18000-32-3]



tetramer

M 235.4

Tetrameric with distorted cubane-like struct., Tl...Tl 384 pm (no direct bond). Synth. from Thallium(*I*) ethoxide, IC-003147 + dry MeOH (1:2).

▷ V. toxic.

Tetramer: Tetra-μ_3-methoxytetrathallium

$C_4H_{12}O_4Tl_4$ M 941.6

Colourless prismatic cryst. (C_6H_6). Sol. C_6H_6, org. solvs. Mp 200° dec.

Dahl, L.F. *et al, J. Inorg. Nucl. Chem.*, 1962, **24**, 357 (*struct, synth*)
Kettle, S.F.A., *Theor. Chim. Acta*, 1966, **4**, 150 (*theory*)
Kurosawa, H. *et al, J. Organomet. Chem.*, 1968, **12**, 241 (*synth*)

CH_3O_4Re IC-002591

(Methoxy)trioxorhenium(*VII*)

(Methoxo)trioxorhenium, 11CI. Methyl perrhenate. Perrhenic acid methyl ester

[44252-75-7]

$MeOReO_3$

M 265.2

Believed to be polymeric. Synth. from ReO_3Cl and Me_3SiOMe in hexane or from $ReO_3(OSiMe_3)$ and Me_3SiOMe in hexane. Colourless prisms, dec. on heating. Sol. THF, chlorinated hydrocarbons; sl. sol. Et_2O; insol. hydrocarbons.

Edwards, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 2695 (*synth, ir, nmr, props*)

IC-002592

$CH_3O_6Zr^{\ominus}$

[Carbonato(2–)-*O*]trihydroxyzirconate(*IV*)(1–), HCl

$[(O_2CO)Zr(OH)_3]^{\ominus}$

M 202.2 (ion)
Tetrahedral anion.
Na salt: [92359-62-1].
Synth. from $Zr(SO_4)_2$ and Na_2CO_3 at controlled pH.
White solid + 2 or 3 H_2O.
H compd.: [88689-79-6]. [*Hydrogen carbonato*-O]*trihydroxyzirconium*(IV). (*Bicarbonato*)*trihydroxyzirconium*(IV)
CH_4O_6Zr M 203.2
Synth. from $Zr(SO_4)_2$ + $NaHCO_3$. White solid.

[92359-62-1]

Samchuk, A.I. *et al*, *Ukr. Khim. Zh. (Russ. Ed.)*, 1983, **49**, 1132 (*synth, H compd*)
Chumakova, L.S. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1984, **29**, 1136 (*synth, ir, thermal dec, powder struct, Na salts*)

IC-002593

$CH_3O_7P_2Tc^{\ominus}$

Hydroxy(methylenediphosphonato)technetate(*IV*)(1–)
(*Methylenediphosphonato*)*oxotechnetium*(IV)

$[Tc(OH)(O_3PCH_2PO_3)]^{\ominus}$

M 287.8 (ion)
This is the one well-characterised species in the Tc-MDP system (See Methylenediphosphonate technetium complex, IC-002517). Each Tc bridges two MDP ligands; each MDP bridges two Tc atoms. Synth. by reaction of $TcBr_6^{2\ominus}$ with MDP.
Li salt: Polymeric solid. Formulated as $([Li(OH_2)_3][Tc(OH)(O_3PCH_2PO_3)]\cdot\frac{1}{3}H_2O)_n$.

Libson, K. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 2476 (*synth, cryst struct*)

IC-002594

$CH_4Cl_4HfN_2O$

Tetrachloro(urea-*O*)hafnium(*IV*), 1HCl
Hafnium(IV) *chloride urea*

[84191-48-0]

$[(H_2N)_2C{=}O]HfCl_4$

M 380.3
Synth. from $HfCl_4$ and excess urea in EtOAc/Et_2O.

Konunova, Ts.B. *et al*, *CA*, 1983, **98**, 45901 (*synth, ir, heat of soln*)

IC-002595

$CH_4Cl_4N_2OZr$

Tetrachloro(urea-*O*)zirconium(*IV*), 1HCl
Zirconium(IV) *chloride urea*

[84191-47-9]

$[(H_2N)_2C{=}O]ZrCl_4$

M 293.0
Synth. from $ZrCl_4$ and urea in EtOAc/Et_2O or EtOAc.

Konunova, Ts.B. *et al*, *Deposited Doc.*, SSPTL, 1981, 784 Khp-D81; *CA*, 1983, **98**, 45901j (*synth, ir, heat of formn*)
Konunova, Ts.B. *et al*, *CA*, 1983, **99**, 168426m.

IC-002596

CH_4N_2O

Ammonium cyanate

$[NH_4][N{=}C{=}O]$

M 60.0
Synth. by reaction of isocyanic acid + anhyd. NH_3. White tetragonal cryst. V. sol. H_2O; sol. EtOH, $CHCl_3$; insol. Et_2O. Rearrs. to urea on heating or prolonged storage.

Inorg. Synth., 1972, **13**, 17; 1976, **16**, 136 (*synth, ir*)

IC-002597

CH_4N_2O

Urea, 9CI, 8CI, USAN
Carbamide. Ureaphil

[57-13-6]

H_2NCONH_2

M 60.0
Constit. of all vertebrate tissues and of many invertebrates. Found esp. in urine. Manuf. on large scale from NH_3 + CO_2 at high press. World prodn. 7.2 mt/a in 1970. Also occurs in many plants in traces and in larger amounts in fungi. Fertiliser, cattle feed supplement, also used in manuf. of urea-formaldehyde resins. Forms clathrates (inclusion complexes) with hydrocarbons. This prop. used in petrochemicals industry. Diuretic, dermatic, keratolytic and antiseptic. Tetragonal needles or prisms with faint salty taste (H_2O or EtOH). V. sol. H_2O, sol. MeOH, EtOH, insol. $CHCl_3$, C_6H_6. Aq. solns hydrol. v. slowly to ammonium carbamate then to NH_3 + CO_2. Weak base. Polymer with formaldehyde (Polynoxylin, BAN, INN) used as a topical antibacterial and antifungal agent.

▷ Mod. toxic. YR6250000.

B,HCl: [506-89-8].
Plates or faintly yellow, deliquescent cryst. Sol. H_2O. Mp 145° dec.
N-*Ac*: [591-07-1]. N-*Aminocarbonylacetamide*, *9CI*
$C_3H_6N_2O_2$ M 102.0
Cryst. Mp 215-216°.
N,N'-*Di-Ac*: N,N'-*Carbonylbisacetamide*, *9CI*
$C_5H_8N_2O_3$ M 144.1
Needles (EtOH). Mp 152-153°.
N,N'-*Dibenzoyl*:
$C_{15}H_{12}N_2O_3$ M 268.2
Needles (Me_2CO or EtOH). Mp 215.5-216.5°.
Cpd. with H_2O_2 (*1:1*): [124-43-6]. ***Carbamide peroxide*, USAN**
Topical antiinfective (dental). Component of Murine.
▷ YT4850000.

[9011-05-6]

Reifer, J. *et al*, *J. Biol. Chem.*, 1949, **178**, 715 (*occur*)
Terss, R.H. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 580 (*deriv*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **21**, 37 (*rev, bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **1**, 455.
Witanowski, M. *et al*, *Tetrahedron*, 1976, **32**, 2127 (*nmr*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 2361.
Swawinathan, S. *et al*, *Acta Crystallogr., Sect. B*, 1984, **40**, 300 (*cryst struct*)
Horsch, W. *et al*, *Pharmazie*, 1985, **40**, 665 (*rev, use, props*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 16, 216.

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 312.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3448.

IC-002598

$CH_4N_2O_2S$

Thiourea *S,S*-dioxide
Formamidinesulfinic acid

[4189-44-0]

$HN{=}C(NH_2)SO_2H$

M 108.1
Exists as zwitterion. Useful for reducing ketones to secondary alcohols. Mp 144° dec.

▷ YU2820000.

Barnett, E.B., *J. Chem. Soc.*, 1910, **97**, 63 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 586 (*use*)

IC-002599

$CH_4N_2O_3S$

Aminoiminomethanesulfonic acid, 9CI
Thiourea S-trioxide. Guanylsulfonic acid

[1184-90-3]

$HN{=}C(NH_2)SO_3H$

M 124.1
Zwitterionic. Cryst. (AcOH). Mp 131-131.5° (112-115°). Stable at 0°.
N-*Me*: [25343-47-9].
$C_2H_6N_2O_3S$ M 138.1
Cryst. Mp 154-156° dec.
N,N-*Di-Me*: [25343-55-9].
$C_3H_8N_2O_3S$ M 152.1
Rhombic cryst. Mp 169-173° dec.
N-*tert-Butyl*: [25343-56-0].
$C_5H_{12}N_2O_3S$ M 180.2
Prisms. Mp 199-202°.
N-*Benzyl*: [101030-88-0].
$C_8H_{10}N_2O_3S$ M 214.2
Cryst. Mp 168° dec.
N-*Ph*: [25343-52-6].
$C_7H_8N_2O_3S$ M 200.2
Solid. Mp 161-161.5° (171-172°).
N,N-*Diisopropyl*: [25348-84-9].
$C_7H_{16}N_2O_3S$ M 208.2
Prisms. Mp 210.5-212° dec.
N,N-*Di-Ph*: [107678-85-3].
$C_{13}H_{12}N_2O_3S$ M 276.3
Cryst. (MeOH/Et_2O). Mp 209-209.5°.

Debowski, Z., *Przem. Chem.*, 1965, **44**, 82; *CA*, **63**, 479 (*synth*)
Walter, W. *et al*, *Justus Liebigs Ann. Chem.*, 1969, **722**, 98 (*deriv, synth*)
Miller, A.E. *et al*, *Synthesis*, 1986, 777 (*synth, ir*)

IC-002600

CH_4N_2S

Ammonium thiocyanate (NH_4SCN)
Ammonium sulfocyanate. Ammonium rhodanide

[1762-95-4]

$[NH_4]SCN$

M 76.1
Prepd. e.g. by boiling aq. NH_4CN with S, by reaction of NH_3 with CS_2, etc. Used as a chem. intermediate, in photography and as a stabilising agent; commercially available. Deliquescent, colourless cryst. Rearranges on heating to an equilib. mixt. with thiourea. V. sol. H_2O, EtOH; sol. MeOH, Me_2CO; prac. insol. $CHCl_3$, EtOAc. Mp 149°.

▷ Poison by ingestion. XK7875000.

Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 372 (*rev*)
Tramer, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1959, **249**, 2755 (*ir, raman*)
Bats, J.W. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1542 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **22**, 156 (*rev*)
Dickson, R.M. *et al*, *Can. J. Chem.*, 1987, **65**, 941 (*cmr, N-15 assn*)
Merck Index, 11th Ed., 1989, No. 591
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 244.

IC-002601

CH_4N_2S

Thiourea, 9CI
Thiocarbamide. Thiocarbonic diamide

[62-56-6]

H_2NCSNH_2

M 76.1
Metab. of *Verticillium albo-atrum* and *Botrytis cinerea*. Also from seeds of *Laburnum anagyroides* and from *Citrus* spp. Photographic fixer. Forms separable inclusion complexes. Used in heterocyclic synth. Used as 10% aq. soln. for photometric detn. of Bi (λ_{max} 470 nm, ε 9000), Os, Ru, Re, Se, Te; reducing agent. Rhombohedra or needles (EtOH). Sol. H_2O, EtOH; spar. sol. Et_2O. Mp 180°.

▷ An exp. carcinogen. YU2800000.

B,HCl: Mp 136-137°.
N-*Ac*: [591-08-2]. N-(*Aminothioxomethyl*)*acetamide*, *9CI*; *1-Acetyl-2-thiourea*, *8CI*
Reagent for synth. of thiols. Needles. Mp 165°.
▷ Severe poison. YR7700000.
N,S-*Di-Ac*:
$C_4H_8N_2O_2S$ M 160.1
Yellow prisms (AcOH aq.). Mp 153°.
S-*Me*: see *Carbamimidothioic acid methyl ester*, IC-003215
N-*Tri-Me*: [2489-77-2].
$C_4H_{10}N_2S$ M 118.2
Prisms (C_6H_6/ligroin). Mp 87-88°.
▷ YU4900000.
N-*Tetra-Et*: [4274-15-1].
$C_9H_{20}N_2S$ M 188.3
Bp 264-266°, Bp_{12} 130°.

U.S. Pat., 2 006 762, (1935); *CA*, 1935, **29**, 5463 (*synth*)
Moore, M.L. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 3273 (*deriv, synth, tox*)
U.S. Pat., 2 337 882, (1944); *CA*, 1944, **38**, 3296 (*synth*)
Allan, W.J. *et al*, *Anal. Chem.*, 1952, **24**, 1608 (*deriv, Os*)
Nielsch, W. *et al*, *Z. Anal. Chem.*, 1954, **142**, 321; **143**, 13, 168 (*deriv, Bi*)
Lisicki, N.M. *et al*, *Anal. Chem.*, 1955, **27**, 1722 (*deriv, Bi*)
Ryabchikov, D.I. *et al*, *Talanta*, 1963, **10**, 13 (*deriv, Re*)
Ger. Pat., 1 957 202, (1971); *CA*, **75**, 151880 (*manuf*)
Kiba, T. *et al*, *Talanta*, 1972, **19**, 451 (*deriv, Ru*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 7; **6**, 586.
Witanowski, M. *et al*, *Tetrahedron*, 1976, **32**, 2127 (*nmr*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 313.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2069.

$CH_4N_2S_2$ IC-002602

Dithiocarbazic acid, 8CI

Hydrazinecarbodithioic acid, 9CI. Dithiocarbazinic acid. Hydrazinodithioformic acid. Aminodithiocarbamic acid. Hythizine

[471-32-9]

$H_2NNHCSSH$

M 108.1

Unknown in free state.

Hydrazine salt. [53636-08-1]

$CH_8N_4S_2$ M 140.2

Prisms. Mp 124° dec.

Me ester. [5397-03-5]

$C_2H_6N_2S_2$ M 122.2

Prisms (C_6H_6). Mp 79°.

Curtius, T. *et al., Ber.*, 1894, **27**, 55 (*salts*)
Sandstrom, J., *Ark. Kemi.*, 1952, **4**, 297; *CA*, **47**, 9271 (*esters*)
Kubota, S. *et al., J. Med. Chem.*, 1978, **21**, 591 (*esters*)
Maites, R. *et al., J. Chem. Soc., Dalton Trans.*, 1980, 423 (*cryst struct, bibl*)
Manogaran, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2628 (*struct, bibl*)
Haines, R.A. *et al., Inorg. Chim. Acta*, 1983, **71**, 1 (*complexes*)
Gattow, G. *et al., Z. Anorg. Allg. Chem.*, 1985, **531**, 101 (*esters, bibl*)

CH_4N_2Se IC-002603

Selenoures, 9CI

[630-10-4]

$(H_2N)_2C{=}Se$

M 123.0

Synth. from H_2Se + cyanamide. Used for photometric detn. of Ru and Os. Prisms or needles (H_2O). Mp 200° dec. (slow heat), Mp 235° dec. Air and light sensitive.

▷ Poison. YU1820000.

B.MeI: Methylisoselenourea iodide

Yellow cryst. Mp 187-188° dec.

B.$MeHSO_4$: Methylisoselenourea hydrogen sulfate

Yellow cryst. Mp 67-70° dec. Structure: $[H_2N{-}C(SeMe){=}NH_2]HSO_4$

N-Me. [5533-49-3]

$C_2H_6N_2Se$ M 137.0

Mp 156-157°

N,N-Di-Me.

$C_3H_8N_2Se$ M 151.0

Mp 98-100°

N,N'-Di-Me. [5533-46-0]

Mp 110-111°

N,N,N',N'-Tetra-Me. [5943-53-3]

$C_6H_{12}N_2Se$ M 179.1

Mp 79-81°

N-Et. [33251-42-2]

Mp 125°

N-Ph. [6124-02-3]

$C_7H_8N_2Se$ M 199.1

Mp 191-192°

N,N-Di-Ph. [21347-28-4]

$C_{13}H_{12}N_2Se$ M 275.2

Mp 205-207° dec.

N,N'-Di-Ph. [16519-43-0]

Mp 178-182° dec. Mp 190-192°

Backer, H.J. *et al., Recl. Trav. Chim. Pays-Bas [J. R. Neth. Chem. Soc.]*, 1943, **62**, 580 (*synth*)
Dunbar, P.E. *et al., J. Am. Chem. Soc.*, 1947, **69**, 1833 (*synth*)
King, L.C. *et al., J. Am. Chem. Soc.*, 1951, **73**, 1864 (*synth*)
Pilipenko, A.T. *et al., Zh. Anal. Khim.*, 1961, **16**, 73
Pilipenko, A.T. *et al., Zh. Neorg. Khim.*, 1961, **6**, 413 (*deriv, Ru, Os*)
Hope, H., *Acta Chem. Scand.*, 1964, **18**, 1800 (*synth*)
Jensen, K.A. *et al., Acta Chem. Scand.*, 1966, **20**, 597 (*deriv*)
Guedicelli, J.F. *et al., Bull. Soc. Chim. Fr.*, 1968, 1099 (*deriv*)
Klayman, D.L. *et al., J. Org. Chem.*, 1969, **34**, 3549 (*deriv*)
Rutherford, J.S. *et al., Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1969, **128**, 229 (*cryst struct*)
Duncan, J.L. *et al., J. Chem. Soc. A*, 1971, 2695 (*ir, raman*)
Walter, W. *et al., Tetrahedron*, 1972, **28**, 3233 (*pmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1978, **D6**, 241 (*bibl*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3015 (*haz*)

CH_4O_3S IC-002604

Methanesulfonic acid, 9CI, 8CI

Methylsulfonic acid. Sulfomethane

[75-75-2]

$MeSO_3H$

M 96.1

Reagent for ester cleavage and removal of *N*-benzyl protecting groups. Solid or liq. Sol. H_2O, EtOH, Et_2O. d_4^{18} 1.48. Mp 20° Bp 122°, Bp_{10} 167.0-167.5°.

▷ Highly irritant, corrosive. PB1140000.

NH_4 salt. Plates. Sol. H_2O

Me ester. [66-27-3]

$C_2H_6O_3S$ M 110.1

Liq. d_4^{25} 1.29. Bp_{753} 203°, $Bp_{0.8}$ 59°.

▷ PB2625000.

Anhydride. [7143-01-3]

$C_2H_6O_5S_2$ M 174.1

Acylating agent. Prisms (Et_2O). Sol. $CHCl_3$, C_6H_6, hot Et_2O. Mp 71°. Bp_{10} 138°.

Chloride. [124-63-0]. *Mesyl chloride*

CH_3ClO_2S M 114.5

Mesylating agent, synthetic intermed. Anal. reagent for monoglycerides. Insol. H_2O. d_4^{18} 1.48. Bp_{750} 161-161.5°; Bp_{18} 62°

Amide. [3144-09-0]

CH_5NO_2S M 95.1

Prisms (H_2O). Mp 88°.

Billeter, O.C., *Ber.*, 1905, **38**, 2015 (*deriv*)
Laumer, P.H. *et al., J. Org. Chem.*, 1940, **5**, 24 (*synth*)
McInnes, A.G., *J. Am. Oil Chem. Assoc.*, 1960, **37**, 7 (*use, chloride*)
Org. Synth., Coll. Vol., 4, 1963, 571 (*chloride*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, 1, 667; **4**, 326; **7**, 225.
Lowe, O.G., *J. Org. Chem.*, 1976, **41**, 2061 (*synth*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 315.
Sax, N.I. *et al., Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2216.

CH_5B IC-002605

Methylborane, 10CI, 9CI, 8CI

Methylborine

[12538-96-4]

$MeBH_2$

M 27.8

Exists as B-H bridged dimer in the uncomplexed state. From $LiMeBH_3$ + HCl. Hydroboration agent. Sequentially adds to alkenes to give mixed boranes RMeBH and RR'MeB. Air- and moisture-sensitive; readily redistributes to other compds. of the type Me_nBH_{3-n}. Sol. non-hydroxylic solvs.

Me_3N complex. [52920-77-1]

Dihydromethyl(trimethylamine)boron. N,N-Dimethylmethanamine methylborane

$C_4H_{14}BN$ M 86.9

Prepd. from $MeBH_3Li$ and NMe_3HCl. Sol. pentane. Mp 0°.

Me_2NH complex. [52920-78-2]. *(Dimethylamine) dihydromethylboran. Dimethylamine methylborane*

$C_3H_{12}BN$ M 72.9

Prepd. by amine exchange of $MeBH_2{\cdot}NMe_3$ with excess Me_2NH. Colourless involatile liq. Sol. $CHCl_3$.

Schlesinger, H.I. *et al., J. Am. Chem. Soc.*, 1939, **61**, 1078 (*deriv*)
Stock, S.J. *et al., J. Phys. Chem.*, 1969, **73**, 1000 (*ms*)
Nöth, H. *et al., Chem. Ber.*, 1974, **107**, 3039 (*nmr*)
Beachley, O.T. *et al., Inorg. Chem.*, 1975, **14**, 120 (*deriv*)
Dill, J.D. *et al., J. Am. Chem. Soc.*, 1976, **98**, 1663 (*struct*)
Pons, A. *et al., J. Comput. Chem.*, 1980, **1**, 295 (*struct*)
Brown, H.C. *et al., J. Org. Chem.*, 1986, **51**, 4925 (*synth, B-11 nmr, ir*)
Strebik, M. *et al., Tetrahedron Lett.*, 1987, **28**, 3771 (*synth, reactions*)

CH_5BF_3N IC-002606

Trifluoro(methylamine)boron

Trifluoroborane methylamine. Boron trifluoride-methylamine compd. (1:1), 8CI. Trifluoroborane-methanamine compd. (1:1), 9CI

[373-56-8]

$F_3B{\cdot}NH_2Me$

M 98.8

Curing agent for epoxy compds. Colourless solid. Sol. EtOH, H_2O; mod. sol. Et_2O; insol. C_6H_6. Mp 66°. Bp_1 158-160°.

Geller, S. *et al., Acta Crystallogr.*, 1950, **3**, 121 (*cryst struct*)
Spitsyn, V.I. *et al., Dokl. Chem. (Engl. Transl.)*, 1965, **160**, 180 (*synth*)
Greenwood, N.N. *et al., J. Chem. Soc. A*, 1966, 21 (*synth, pmr, B-11 nmr, F-19 nmr*)
Delaule, J. *et al., Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1967, **265**, 849 (*ir*)
Schanck, A. *et al., Adv. Mol. Relax. Processes*, 1975, **7**, 149 (*dta, pmr, F-19 nmr solid state*)
Smith, R.E. *et al., J. Appl. Polym. Sci.*, 1984, **29**, 3697 (*use*)

CH_5BN_2 IC-002607

Ammine(cyano-*C*)dihydroboron, 10CI, 9CI

Cyanoborane ammonia. Boranecarbonitrile monoammoniate, 9CI

[59301-48-3]

$H_3N{-}BH_2CN$

M 55.8

White solid. Mp 89°.

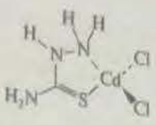
Bratt, P.J. *et al., J. Chem. Soc., Dalton Trans.*, 1976, 353 (*synth, ir*)
McPhail, A.T. *et al., J. Chem. Res. (S)*, 1978, 205 (*cryst struct*)
Hall, I.H. *et al., J. Pharm. Sci.*, 1980, **69**, 1025; 1981, **70**, 339 (*pharmacol*)

$CH_5CdCl_2N_3S$ IC-002608

Dichloro(hydrazinecarbothioamide-N^2,*S*)cadmium, 10CI

Dichloro(thiosemicarbazide)cadmium. (Thiosemicarbazide) cadmium dichloride

[66082-97-1]



M 274.4

Monohydrate. [68934-12-3]

Non-linear optical material. Needles (H_2O). Dehydrates at 140°, dec. at 230°. Struct. polymeric with octahedral Cd; H_2O not coordinated to metal.

[99145-21-8, 117619-46-2]

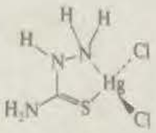
Nardelli, M. *et al., Ric. Sci.*, 1960, **30**, 276 (*synth*)
Murzubraimov, B., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 309, 1728 (*phase diagram*)
Murzubraimov, B. *et al., Koord. Khim.*, 1985, **11**, 596 (*ir*)
Woode, M.K. *et al., Acta Crystallogr., Sect. C*, 1987, **43**, 2324 (*cryst struct*)
Tao, X. *et al., CA*, 1987, **107**, 186679 (*struct, optical props*)
Wang, J. *et al., CA*, 1988, **109**, 179430 (*raman*)
Xu, D. *et al., CA*, 1988, **109**, 218913 (*cryst struct, thermal anal*)

$CH_5Cl_2HgN_3S$ IC-002609

Dichloro(hydrazinecarbothioamide-N^2,*S*)mercury(*II*), 10CI

(Thiosemicarbazide)dichloromercury(II)

[65531-88-6]



M 362.6

Needles (aq. EtOH). Isostructural with corresp. bromide.

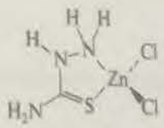
Chieh, C. *et al., Can. J. Chem.*, 1977, **55**, 3898; 1978, **56**, 2526 (*synth, cryst struct, pmr, ir, raman*)

$CH_5Cl_2N_3SZn$ IC-002610

Dichloro(hydrazinecarbothioamide-N^2,*S*)zinc(*II*), 10CI

Dichloro(thiosemicarbazide)zinc. Thiosemicarbazidezinc dichloride

[52281-94-4]



M 227.4

Tetrahedral Zn. Needles (H_2O). Mp 240°.

Cavalca, L. *et al., Acta Crystallogr.*, 1960, **13**, 688 (*cryst struct*)
Nardelli, M. *et al., Ric. Sci.*, 1960, **30**, 276 (*synth*)
Adejumbi, A. *et al., J. Inorg. Nucl. Chem.*, 1977, **39**, 910 (*ir*)
Shtrempler, G.I. *et al., Zh. Neorg. Khim.*, 1982, **27**, 789 (*thermal props*)
Mirzubaimov, B. *et al., Koord. Khim.*, 1985, **11**, 596 (*ir*)

CH_3NNiO_4 IC-002611

Dihydroxy(methoxy)nitrosylnickel

Dihydroxo(methoxo)nitrosylnickel

$[Ni(NO)(OH)_2(OMe)]$

M 153.7

Probably tetrahedral monomer with Ni(*II*) and $NO^{\ominus}$.

From $Ni(CO)_4$ + NO in MeOH.

Griffith, W.P. *et al, J. Chem. Soc.*, 1959, 1775

$CH_4B^{\ominus}$ IC-002612

Trihydromethylborate(1 –)

Methylborohydride

[71844-38-7]

$[MeBH_3]^{\ominus}$

M 28.8 (ion)

Li salt: [52950-75-1].

CH_6BLi M 35.8

Air- and moisture-sensitive.

Mg salt: [68193-75-9]. *Bis[trihydromethylborato(1 –)-H,H']magnesium*

$C_2H_{12}B_2Mg$ M 82.0

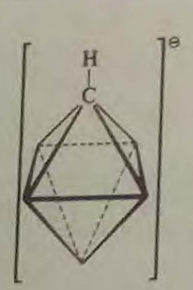
Air- and moisture-sensitive.

Goel, A.B., *Indian J. Chem., Sect. A*, 1978, **16**, 491.
Umeyama, H. *et al, Chem. Pharm. Bull.*, 1979, **27**, 1626 (*props*)
Prosx, A. *et al, Tetrahedron*, 1980, **36**, 673 (*props*)
Biffar, W. *et al, Chem. Ber.*, 1981, **114**, 49 (*nmr*)

$CH_4B_5^{\ominus}$ IC-002613

Hexahydro-1-carbahexaborate(1 –), 11Cl, 9Cl

[96333-13-0]



M 72.1 (ion)

closo-.

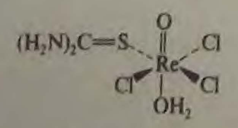
Na salt: Colourless solid. Sol. THF.

Prince, S.R. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 451 (*synth, B-11 nmr*)

$CH_6Cl_3N_2O_2ReS$ IC-002614

Aquatrichlorooxo(thiourea-*S*)rhenium(*V*), 10Cl

[62390-35-6]



mer,trans-form

M 402.7

mer,trans-form

Interatomic distance: Re=O 171 pm. Synth. from NH_4ReO_4 or $KReO_4$ and thiourea in conc. HCl. Green cryst.

Lis, T., *Acta Crystallogr., Sect. B*, 1977, **33**, 944 (*synth, cryst struct*)

$CH_6CuN_2O_3$ IC-002615

Diammine[carbonato(2 –)-*O,O'*]copper, 10Cl

Diamminecopper(II) carbonate.

Carbonatodiamminecopper(II)

[36119-84-3]

$Cu(NH_3)_2(CO_3)$

M 157.6

Struct. consists of square pyramidally coordinated copper ions, held together in layers by hydrogen bonds. There are superexchange interactions. Dark blue cryst. Dec. by moist air.

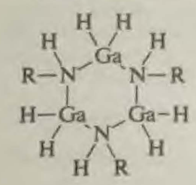
[21710-50-9]

Tomlinson, A.A.G. *et al, J. Chem. Soc. A*, 1968, **10**, 2578 (*rev, synth, ir, ue, esr*)
Meyer, M.H. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 1607 (*synth, cryst struct*)
Jeter, D.Y. *et al, Inorg. Chem.*, 1972, **11**, 185 (*synth, magnetism*)
Ouahes, R. *et al, Rev. Chim. Minér.*, 1972, **9**, 309; *CA*, **77**, 96349 (*synth, ir, magnetism*)
Kamase, K. *et al, Inorg. Chem.*, 1978, **17**, 2958 (*magnetism*)
Gregson, A.K. *et al, Inorg. Chem.*, 1980, **19**, 3436 (*magnetism*)

CH_6GaN IC-002616

Dihydro(methylamido)gallium(*III*)

(Methylaminato)dihydrogallium(III)



trimer

R = Me

M 101.7

Trimeric. Compds. with other amides also reported.

Trimer: [22357-77-3]. *Hexahydrotris(μ-methylaminato)trigallium*

$C_3H_{18}Ga_3N_3$ M 305.3

Synth. from Me_3NGaH_3 and NMe_2H. Sticky air- and moisture-sensitive solid. Sol. C_6H_6. Isomers detected in soln. by nmr.

Storr, A. *et al, J. Chem. Soc. A*, 1968, 2605; 1971, 1237 (*synth, nmr, ir*)

CH_6GeS IC-002617

(Methylthio)germane, 9Cl

(Methanethiolato)germane. Germyl methyl sulfide

[16643-16-6]

H_3GeSMe

M 122.7

Volatile liq. Mp –97°. Bp 87° (extrap.).

Wang, J.T. *et al, Inorg. Chem.*, 1968, **7**, 1319 (*synth, ir, ms, pmr*)
Cradock, S., *J. Chem. Soc. A*, 1968, 1426 (*ir, raman*)
Inorg. Synth., 1978, **18**, 161 (*synth*)
Drake, J.E. *et al, Spectrochim. Acta, Part A*, 1982, **38**, 31 (*ir, raman*)

CH_4NO_2P IC-002618

Methylphosphoramidous acid, 9Cl

Dihydroxo(methylamido)phosphorus(III)

$MeNHP(OH)_2$

M 95.0

Tautomeric.

Di-Me ester: [39480-85-8]. *Dimethyl methylphosphoramidite*

$C_3H_{10}NO_2P$ M 123.0

Liq. Bp_{16} 43-46°.

Di-Et ester: [60030-06-0]. *Diethyl methylphosphoramidite*

$C_5H_{14}NO_2P$ M 151.1

Liq. Bp_{10} 53-55°. n_D^{20} 1.4295.

Diisopropyl ester: Diisopropyl methylphosphoramidite

$C_7H_{18}NO_2P$ M 179.1

Liq. Bp_{12} 63.5°. n_D^{20} 1.4288.

Difluoride: [2851-75-4].

CH_4F_2NP M 99.0

Ligand for Co, Fe, W, and Mo. Liq. Bp 52-53° dec.

Barlow, C.G. *et al, J. Chem. Soc. A*, 1968, 2692 (*difluoride, synth, props, ir, pmr, F-19, P-31 nmr*)
Harman, J.S. *et al, J. Chem. Soc. A*, 1970, 1935 (*difluoride*)
Scherer, O.J. *et al, Z. Naturforsch., B*, 1972, **27**, 1429 (*dimethyl ester, synth, pmr*)
Nikonorova, L.K. *et al, Zh. Obshch. Khim.*, 1976, **46**, 1015; *J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 1012 (*esters*)
Laurenson, G.S. *et al, J. Mol. Struct.*, 1979, **54**, 111 (*difluoride, ed*)
Al-Rawi, J.M.A. *et al, Org. Magn. Reson.*, 1984, **22**, 336 (*dimethyl ester, cmr*)

$CH_6N_2O_3$ IC-002619

Ammonium carbamate

Carbamic acid ammonium salt

$[NH_4][H_2NCO_2]$

M 78.0

Formed by reaction of NH_3 (liq.) and CO_2 (solid). White cryst., sl. volatile at 20° and completely dissoc. at 59°. Hydrates to $(NH_4)_2CO_3$. V. sol. H_2O.

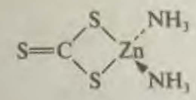
Inorg. Synth., 1964, **2**, 85 (*synth*)

$CH_6N_2S_3Zn$ IC-002620

Diammine[carbonotrithioato(2 –)-*S,S'*]zinc

Diammine(trithiocarbonato)zinc

[15244-60-7]



M 207.6

Possibly dimeric. Cryst. Dec. at 50°.

Dimer: [51435-88-2]. *Tetraamminebis[μ-[carbonotrithioato(2 –)-S:S']]dizinc*

$C_2H_{12}N_4S_6Zn_2$ M 415.3

Hofmann, K.A., *Z. Anorg. Allg. Chem.*, 1897, **14**, 263 (*synth*)
Krebs, B. *et al, Z. Naturforsch., A*, 1965, 1664 (*ir*)
Shul'man, V.M. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 1024 (*synth, thermal anal*)
Ehrhardt, H. *et al, Z. Naturforsch., B*, 1972, **27**, 1104.
Müller, A. *et al, Z. Anorg. Allg. Chem.*, 1973, **401**, 274 (*synth, ir, raman, powder struct*)

$CH_4N_2Si_2$ IC-002621

Disilyl carbodiimide

N,N'-Methanetetraylbis(silanamine), 9Cl

[4468-88-6]

$H_3SiN{=}C{=}NSiH_3$

M 102.2

Originally thought to be Disilylcyanamide ($(H_3Si)_2NCN$). Synth. from SiH_3I + AgNCNAg. Liq. Stable at r.t. for days in sealed apparatus. Mp –74.8°. Bp 84.7°.

Ebsworth, E.A.V. *et al, J. Chem. Soc.*, 1961, 4879 (*synth, props*)
Ebsworth, E.A.V. *et al, Spectrochim. Acta*, 1963, **19**, 1127 (*ir, raman, struct*)
Glidewell, C. *et al, Chem. Phys. Lett.*, 1974, **28**, 290 (*struct*)
Glidewell, C., *Inorg. Nucl. Chem. Lett.*, 1974, **10**, 39 (*synth*)

CH_6N_4S IC-002622

Thiocarbohydrazide, 8Cl

Carbonothioic dihydrazide, 9Cl. Thiocarbazide. Thiocarbonic dihydrazide

[2231-57-4]

$H_2NNHCSNHNH_2$

M 106.1

Cryst. (H_2O). Dec. at 170°.

▷ FF2975000.

1,5-Di-Ac:

$C_5H_{10}N_4O_2S$ M 190.2

Hygroscopic cryst. Mp 204-205°

1-Ph: [2550-71-2].

$C_7H_{10}N_4S$ M 182.2

Tablets (EtOH). Sol. EtOH, AcOH, Py, spar. sol. Me_2CO, $CHCl_3$, C_6H_6.

1-Ph; B,HCl: Plates. Mp 181°.

1-Me, 1-Ph:

$C_8H_{12}N_4S$ M 196.2

Prisms (EtOH). Mp 228-229° dec.

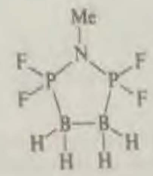
Guha, P.C. *et al, J. Chem. Soc.*, 1924, 1215 (*synth*)
Burns, G.R., *Inorg. Chem.*, 1968, **7**, 277 (*synth*)
Braibanti, A. *et al, J. Chem. Soc., Perkin Trans. 2*, 1972, 2116 (*cryst struct*)

$CH_7B_2F_4NP_2$ IC-002623

2,2,5,5-Tetrafluoro-1-methyl-1,2,5,3,4-azadiphosphadiborolidine

Methylaminobis(difluorophosphino)diborane(4). Diborane, compd. with methylimidodiphosphoroustetrafluoride (1:1), 10Cl

[63228-80-8]



M 192.6

Unusual B_2P_2N ring. Unstable at r.t.

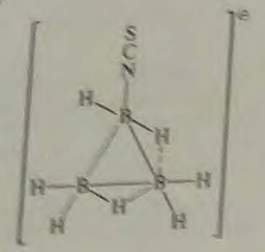
Paine, R.T., *J. Am. Chem. Soc.*, 1977, **99**, 3884 (*synth, ms, ir, pmr, B-11 nmr, F-19 nmr*)

$CH_2B_3NS^{\ominus}$ IC-002624

1-Isothiocyanatoheptahydrotriborate(1−)

Heptahydro-3-(thiocyanato-N)triborate(1−)

[82404-60-2]



M 97.5 (ion)

Bis(triphenylphosphine)iminium salt. [82404-62-4]

Synth. from $[(Ph_3P)_2N]B_3H_8Cl$ + AgSCN. White cryst. (CH_2Cl_2).

Morris, J.H. *et al, Inorg. Chim. Acta*, 1982, **59**, 207; 1985, **103**, 51 (*synth, ir, pmr, B-11 nmr*)

Andrews, S.J. *et al, Inorg. Chim. Acta*, 1984, **88**, 153 (*cryst struct*)

Morris, J.H. *et al, Polyhedron*, 1986, **5**, 1859 (*B-11 nmr*)

CH_2B_5 IC-002625

1-Carbahexaborane(7), 10Cl

1-Carbahexaborane(7)-2,3,6-μ3-H

[55188-36-8]

M 73.1

Exopolynal chloro-. Colourless liq. by vacuum fractionation.

Grosszek, E. *et al, Inorg. Chem.*, 1971, **10**, 2770 (*synth, nmr*)

Onak, T. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 76 (*nmr*)

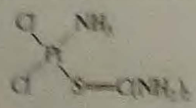
Onak, T. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 665

McNeill, E.A. *et al, Inorg. Chem.*, 1975, **13**, 1083 (*ed*)

McKown, G. *et al, J. Am. Chem. Soc.*, 1976, **98**, 5009 (*microwave*)

$CH_4Cl_2N_2PtS$ IC-002626

Amminedichloro(thiourea)platinum(II)



M 359.1

Probable intermed. in much studied substitution of thiourea into Diamminedichloroplatinum(II). IC-016843, but not ind. No recent studies.

Socrates, I. *et al, Comprr. Coord. Chem.*, Pergamon, Oxford, 1987, **5**, 480 (*rev*)

CH_4BN IC-002627

Trihydro(methylamine)boron

Trihydro(methanamine)boron, 10Cl. Methanamine compd. with borane (1:1), 9Cl. Methylamine compd. with borane, 8Cl. Borane methylamine

[1722-33-4]

$$MeNH_2{-}BH_3$$

M 44.8

Solid. Mp 56°. Dipole moment 5.19D.

Nöth, H. *et al, Chem. Ber.*, 1960, **93**, 928 (*synth*)

Heitsch, C.W., *Inorg. Chem.*, 1965, **4**, 1019 (*nmr*)

Lloyd, D.R. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 947 (*pe*)

Nöth, H. *et al, Chem. Ber.*, 1974, **107**, 3070 (*nmr*)

Umeyama, H. *et al, J. Am. Chem. Soc.*, 1976, **98**, 7208.

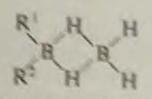
Van Paasschen, J.M. *et al, Inorg. Chem.*, 1978, **17**, 3302.

CH_4B_2 IC-002628

Methyldiborane(6), 10Cl, 9Cl, 8Cl

Monomethyldiborane

[23777-55-1]



$R^1 = Me$, $R^2 = H$

M 41.6

Gas; sensitive to air and moisture; unstable towards disproportionation. Sol. ethers.

Seely, G.R. *et al, Anal. Chem.*, 1959, **31**, 1993 (*chromatog*)

Shapiro, I. *et al, Adv. Chem. Ser.*, 1961, **32**, 127 (*mol*)

Kapshtal, V.N. *et al, Zh. Fiz. Khim.*, 1966, **40**, 2818; *C.A.*, **66**, 80525h (*ir*)

Carpenter, J.H. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 881 (*raman*)

Leach, J.B. *et al, J. Magn. Reson.*, 1972, **6**, 74 (*pmr*)

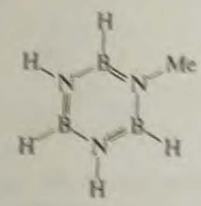
Penn, R.E. *et al, J. Chem. Phys.*, 1977, **67**, 831 (*microwave*)

$CH_4B_2N_2$ IC-002629

1-Methylborazine, 10Cl, 9Cl, 8Cl

1-Methylborazole

[21127-94-6]



M 94.5

Stable compound. V.p. 27 mm at r.t., 23.5 mm at 0°.

Hoffmann, R., *J. Chem. Phys.*, 1964, **40**, 2474 (*struct*)

Powell, P. *et al, J. Chem. Soc.*, 1964, 280 (*synth*)

Beachley, O.T., *Inorg. Chem.*, 1969, **8**, 981 (*nmr, ms, ir*)

Boussaleou, G. *et al, Org. Magn. Reson.*, 1973, **5**, 585 (*nmr*)

Turbini, L.J. *et al, Org. Magn. Reson.*, 1974, **6**, 450 (*pmr*)

Kline, G.A. *et al, Inorg. Chem.*, 1977, **16**, 11 (*props, nmr*)

$CH_4CdN_2O_4S_2$ IC-002630

Diaquasulfato(thiourea)cadmium

(Thiourea)cadmium sulfate dihydrate

[50704-66-6]

$$(H_2O)_2Cd[S{=}C(NH_2)_2](SO_4)$$

M 320.6

Polymeric chain struct. with octahedral Cd and bridging thiourea and sulfate ligands. Cryst.

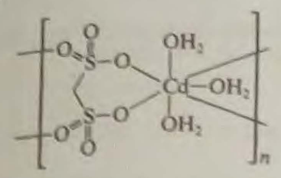
Nardelli, M. *et al, Ric. Sci.*, 1958, **28**, 1016 (*synth*)

Cavalca, L. *et al, Acta Crystallogr.*, 1967, **22**, 878 (*cryst struct*)

$CH_4CdO_8S_2$ IC-002631

Triaqua[methanedisulfonato(2−)]cadmium(II)

[74522-78-4]



Solid state struct.

M 340.6

3-Coordinate infinite chain struct. in solid state. Cryst. (H_2O). Mp 410° dec. Dehydrates on heating to anhydrous salt. Dec. on melting to CdS.

Charbonnier, F. *et al, Rev. Chim. Minér.*, 1979, **16**, 555 (*synth, cryst struct, thermal anal*)

$CH_2Mg_5O_8$ IC-002632

Magnesium carbonate dihydroxide trihydrate

Basic magnesium carbonate trihydrate

$$Mg_5(CO_3)(OH)_2{\cdot}3H_2O$$

M 196.6

Mineral. White monoclinic cryst. Dec. on heating with loss of CO_2 and H_2O.

Mineral-form [12143-96-3]

Artinite

Occur. assoc. with various Mg-bearing minerals. White fibrous cryst.

Jagodzinski, H., *Mineral. Petrogr. Mitt.*, 1965, **10**, 297 (*cryst struct*)

Hirotsu, S. *et al, CA*, 1978, **89**, 190234 (*ir, dta*)

$CH_8N_2O_3$ IC-002633

Ammonium carbonate ($(NH_4)_2CO_3$)

Carbonic acid, ammonium salt. Diammonium carbonate. Sal volatile. Hartshorn

[506-87-6]

$$(NH_4)_2CO_3$$

M 96.0

Mixt. of ammonium carbamate and ammonium carbonate. Synth. from aq. NH_3 + CO_2. Commercially available. Used in baking powders, in tanning, as dye mordant, in manuf. rubber articles, casein glue, smelling salts, fire extinguishers, as analytical reagent, as source of NH_3 (pharmaceut.) and as an expectorant. Colourless cryst. Strong odour of NH_3. Sharp taste. V. sol. H_2O. Mp 58° dec. Dec. in air → NH_3 + CO_2 + H_2O. Converts to ammonium bicarbonate.

▶ BP 952000.

Waller Compr. Treat. Inorg. Theor. Chem., Longman, London, 1964, **8**(**1A**), 459 (*rev*)

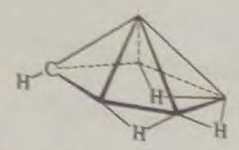
Merck Index, 10th Ed., 1983, No. 519 (*props*)

Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 233 (*haz*)

CH_9B_5 IC-002634

2-Carbahexaborane(9), 10Cl

[12385-35-2]



M 75.1

nido-. Colourless liq. by vacuum fractionation.

Dunks, G. *et al, Inorg. Chem.*, 1969, **8**, 2667 (*synth, nmr, ir*)

Cheung, C. *et al, Inorg. Chem.*, 1971, **10**, 1144 (*microwave struct*)

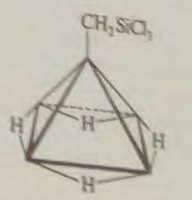
Grosszek, E. *et al, Inorg. Chem.*, 1971, **10**, 2770 (*synth*)

Leach, J.B. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 819 (*synth*)

$CH_{10}B_5Cl_3Si$ IC-002635

1-[(Trichlorosilyl)methyl]pentaborane(9), 10Cl

[63788-21-6]



M 210.5

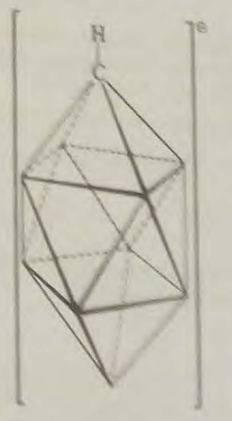
Synth. from reaction of B_5H_9 and $Si(CH_2Cl)Cl_3$ with $AlCl_3$ catalyst at 90° followed by cold column fractionation between −25 and +20°. Colourless liq. assumed to be moisture sensitive.

Leach, J.B. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 819 (*nmr, ms, synth*)

$CH_{10}B_9^{\ominus}$ IC-002638

Decahydro-1-carbadecaborate(1−), 11Cl, 9Cl, 8Cl

[45730-70-9]



M 119.3 (ion)

closo-

Cs salt: [12539-20-7]

$CH_{10}B_9Cs$ M 252.2

Colourless solid. Sol. MeCN.

Me_4N salt: [12546-54-2]

Colourless solid. Sol. MeCN.

Knoth, W.H., *J. Am. Chem. Soc.*, 1967, **89**, 1274 (*synth, h. pmr, B-11 nmr*)

Knoth, W.H., *Inorg. Chem.*, 1971, **10**, 598 (*synth, ir, pmr, B-11 nmr*)
Wiersma, R.J. *et al, Inorg. Chem.*, 1973, **12**, 785 (*B-11 nmr, electrochem*)

IC-002637

$CH_{10}CrNO_5S^{2\oplus}$

Pentaaqua(thiocyanato-*S*)chromium(*III*)(2+), 11Cl, 9Cl

[22258-88-4]

$[Cr(SCN)(OH_2)_5]^{2\oplus}$

M 200.1 (ion)
Bis-Me_4N Salt: Formed in soln.; not isol.
Orhanović, M. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4286 (*kinetics*)

IC-002638

$CH_{10}FeNO_5S^{2\oplus}$

Pentaaqua(isothiocyanato)iron(*II*)(2+)
Pentaaqua(thiocyanato-N)iron(2+), 11Cl

[23724-08-5]

$[Fe(NCS)(OH_2)_5]^{2\oplus}$

M 204.0 (ion)
Species which gives rise to blood red colour with Fe(*III*) and $NCS^{\ominus}$ ions in aq.soln. Used in Fe(*III*) qualitative and quantitative anal. Blood red.

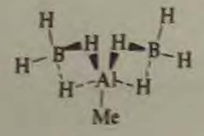
Vogel's Textbook of Quantitative Inorganic Analysis, 4th Ed., Longman, London, 1954, 741 (*use*)
Goodall, D.M. *et al, Sch. Sci. Rev.*, 1981, **63**, 302 (*synth, equil*)
Martinez, P. *et al, Ber. Bunsenges. Phys. Chem.*, 1985, **89**, 728 (*hydrol, soln equil*)

IC-002639

$CH_{11}AlB_2$

Methylbis(tetrahydroborato)aluminium
Methylaluminium bis(tetrahydroborate)

[60257-33-2]



M 71.7
Monomeric. Mp −76°. Extremely sensitive to traces of oxygen or moisture. Forms adducts with NMe_3, PMe_3, $AsMe_3$, Me_2O, Et_2O, Me_2S, Me_2NH.

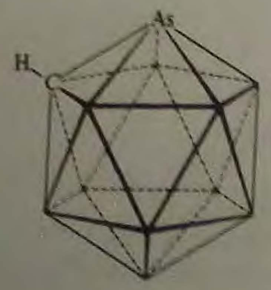
Oddy, P.R. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 869 (*synth, ir*)
Barlow, M.T. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1374 (*synth, struct*)

IC-002640

$CH_{11}AsB_{10}$

1-Arsa-2-carbadodecaborane(11), 10Cl, 9Cl, 8Cl
1,2-Carbaarsenadodecaborane(11)

[23231-66-5]



M 206.1
closo-. Colourless solid. Sol. pet. ether, THF, C_6H_6, CS_2, Me_2CO, DMSO. Mp 399-399.5°.

Todd, L.J. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3376 (*synth, B-11 nmr, ms*)
Todd, L.J. *et al, Inorg. Chem.*, 1970, **9**, 2175 (*synth, ir, pmr, B-11 nmr, ms, props*)
Vinogradova, L.E. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1972, **21**, 2372 (*ir, raman*)

IC-002641

$CH_{11}AsB_{10}$

1-Arsa-7-carbadodecaborane(11), 10Cl, 9Cl, 8Cl
1,7-Carbaarsenadodecaborane(11)

[28965-28-8]

M 206.1
closo-. Colourless solid. Sol. C_6H_6, Me_2CO, DMSO. Mp 351-352°.

Todd, L.J. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3376 (*synth*)
Todd, L.J. *et al, Inorg. Chem.*, 1970, **9**, 2175 (*synth, ir, pmr, B-11 nmr, ms*)
Vinogradova, L.E. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1972, **21**, 2372 (*ir, raman*)

IC-002642

$CH_{11}AsB_{10}$

1-Arsa-12-carbadodecaborane(11), 10Cl, 9Cl, 8Cl
1,12-Carbaarsenadodecaborane(11)

[23151-49-7]

M 206.1
closo-. Colourless solid. Sol. C_6H_6, CS_2, Me_2CO, DMSO. Mp 335-337°.

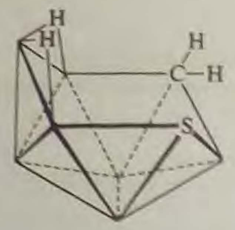
Todd, L.J. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3376 (*synth, B-11 nmr, ms*)
Todd, L.J. *et al, Inorg. Chem.*, 1970, **9**, 2175 (*synth, ir, pmr, B-11 nmr, ms*)
Vinogradova, L.E. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1972, **21**, 2372 (*ir, raman*)

IC-002643

$CH_{11}B_7S$

6-Thia-8-carbanonaborane(11), 10Cl
6,8-Carbathianonaborane(11)

[63115-78-6]



M 130.8
Colourless solid. Sol. org. solvs. Mp 108-110°.

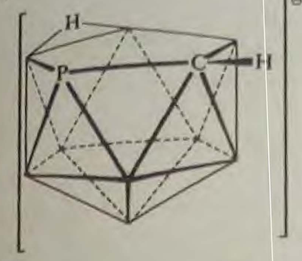
Plesek, J. *et al, Collect. Czech. Chem. Commun.*, 1977, **42**, 785 (*synth, pmr, B-11 nmr, ms, uv*)

IC-002644

$CH_{11}B_9P^{\ominus}$

Undecahydro-7-phospha-8-carbaundecaborate(1−), 9Cl, 8Cl
Undecahydrocarbaphosphaundecaborate(1−)

[52110-38-0]



M 151.3 (ion)
nido-. The 7,9-isomer is also known.
Me_4N salt: [39395-07-8].
Colourless cryst. (MeOH aq.). Sol. Me_2CO.
Piperidinium salt: Colourless cryst. (MeOH aq.). Sol. Me_2CO, DMSO. Mp 296-297°.

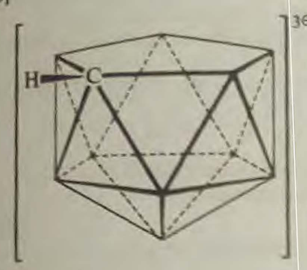
Todd, L.J. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4489 (*synth, ir, pmr*)
Todd, L.J. *et al, Inorg. Chem.*, 1969, **8**, 1698 (*synth, ir, pmr, B-11 nmr*)

IC-002645

$CH_{11}B_{10}^{3\ominus}$

Undecahydro-7-carbaundecaborate(3−), 11Cl, 9Cl

[54183-26-5]



M 131.2 (ion)
nido-.
Tri-Na salt: [51391-29-8].
$CH_{11}B_{10}Na_3$ M 200.1
White solid + 1.8THF. Pyrophoric in moist air.

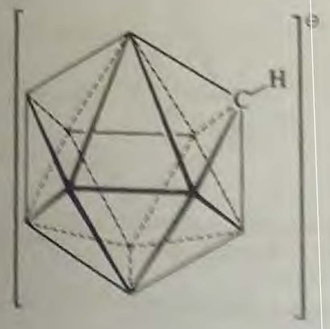
Hyatt, D.E. *et al, Inorg. Chem.*, 1967, **6**, 2229 (*synth*)
Hyatt, D.E. *et al, J. Am. Chem. Soc.*, 1967, **89**, 3342 (*synth*)

IC-002646

$CH_{11}B_{10}^{\ominus}$

Undecahydro-2-carbaundecaborate(1−), 11Cl, 10Cl, 9Cl

[12539-21-8]



M 131.2 (ion)
closo-.
Na salt:
$CH_{11}B_{10}Na$ M 154.1
Colourless solid. Sol. THF, Me_2CO.
Me_4N salt: [12546-58-6].
Colourless solid ($MeOH/Me_2CO$). Sol. Me_2CO.

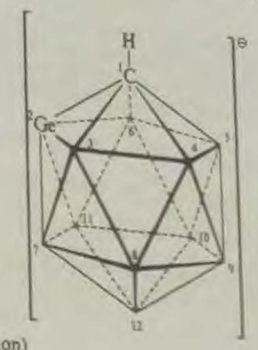
Hyatt, D.E. *et al, Inorg. Chem.*, 1967, **6**, 2229 (*synth, ir, uv, pmr, B-11 nmr*)
Wiersma, R.J. *et al, Inorg. Chem.*, 1973, **12**, 785 (*B-11 nmr, electrochem*)

IC-002647

$CH_{11}B_{10}Ge^{\ominus}$

Undecahydro-1-carba-2-germadodecaborate(1−), 8Cl

[51150-05-1]



M 203.8 (ion)
closo-.
Me_4N salt: [25948-44-1].
Cryst. ($MeOH/Me_2CO$). Sol. Me_2CO, DMSO.

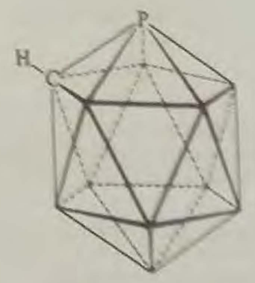
Todd, L.J. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3376 (*synth, ir, pmr, B-11 nmr*)
Wikholm, G.S. *et al, J. Organomet. Chem.*, 1974, **71**, 219 (*synth, ir, pmr, B-11 nmr*)

IC-002648

$CH_{11}B_{10}P$

1-Phospha-2-carbadodecaborane(11), 9Cl, 8Cl
1,2-Carbaphosphadodecaborane(11)

[30112-97-1]



M 162.1
closo-. Colourless solid. Sol. C_6H_6, MeCN, CCl_4, DMSO. Mp 353.5-354.5°.

Little, J.L. *et al, J. Am. Chem. Soc.*, 1967, **89**, 5495 (*synth, B-11 nmr*)
Todd, L.J. *et al, Inorg. Chem.*, 1969, **8**, 1698; 1970, **9**, 2175 (*synth, ir, pmr, B-11 nmr, uv, ms*)
Zakharkin, L.I. *et al, Zh. Obshch. Khim.*, 1971, **41**, 2052 (*electrochem*)
Vinogradova, L.E. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1972, **21**, 2372 (*ir, raman*)
Siedle, A.R. *et al, Inorg. Chem.*, 1974, **13**, 2321 (*pmr, B-11 nmr*)

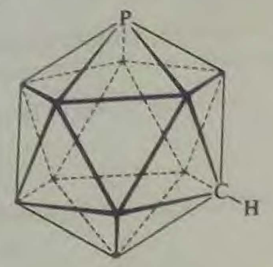
IC-002649

$CH_{11}B_{10}P$

1-Phospha-7-carbadodecaborane(11), 9CI, 8CI

1,7-Carbaphosphadodecaborane(11)

[17398-92-4]



M 162.1

closo-. Obt. by thermally induced isom. of 1-Phospha-2-carbadodecaborane(11), IC-002648. Colourless cryst. (hexane). Sol. MeCN, CCl_4, C_6H_6, DMSO. Mp 325-327°.

Little, J.L. *et al, J. Am. Chem. Soc.*, 1967, **89**, 5495 (*synth, B-11 nmr*)

Todd, L.J. *et al, Inorg. Chem.*, 1969, **8**, 1698; 1970, **9**, 2175 (*synth, ir, pmr, B-11 nmr, uv, ms*)

Zakharkin, L.I. *et al, Zh. Obshch. Khim.*, 1971, **41**, 2052 (*electrochem*)

Vinogradova, L.E. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1972, **21**, 2372 (*ir, raman*)

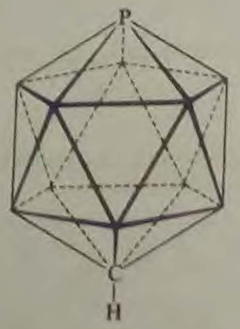
IC-002650

$CH_{11}B_{10}P$

1-Phospha-12-carbadodecaborane(11), 10CI, 9CI, 8CI

1,12-Carbaphosphadodecaborane(11)

[23151-44-2]



M 162.1

closo-. Obt. by thermally induced isom. of 1-Phospha-2-carbadodecaborane(11), IC-002648. Colourless cryst. (pentane). Sol. MeCN, CS_2, CCl_4, DMSO. Mp 314-315.5°.

Todd, L.J. *et al, Inorg. Chem.*, 1969, **8**, 1698 (*synth, ir, pmr, B-11 nmr, ms*)

Zakharkin, L.I. *et al, Zh. Obshch. Khim.*, 1971, **41**, 2052 (*electrochem*)

Vinogradova, L.E. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1972, **21**, 2372 (*ir, raman*)

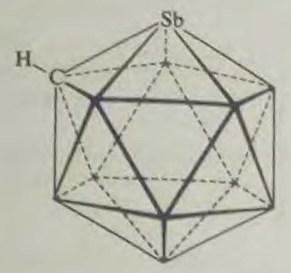
IC-002651

$CH_{11}B_{10}Sb$

1-Stiba-2-carbadodecaborane(11), 8CI

1,2-Carbastibadodecaborane(11)

[28883-32-1]



M 252.9

closo-. Colourless cryst. (C_6H_6). Sol. C_6H_6, CS_2, Me_2CO. Dec. without melting > 240°.

Todd, L.J. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3376 (*synth, B-11 nmr, ms*)

Todd, L.J. *et al, Inorg. Chem.*, 1970, **9**, 2175 (*synth, ir, pmr, B-11 nmr, ms, props*)

IC-002652

$CH_{11}B_{10}Sb$

1-Stiba-7-carbadodecaborane(11), 8CI

1,7-Carbastibadodecaborane(11)

[23231-67-6]

M 252.9

closo-. Colourless solid. Sol. C_6H_6, Me_2CO. Mp 403.5-404.5°.

Todd, L.J. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3376 (*synth, B-11 nmr, ms*)

Todd, L.J. *et al, Inorg. Chem.*, 1970, **9**, 2175 (*synth, ir, pmr, ms*)

IC-002653

$CH_{11}B_{10}Sb$

1-Stiba-12-carbadodecaborane(11)

1,12-Carbastibadodecaborane(11)

M 252.9

closo-. Not isol. Detected by g.l.c.

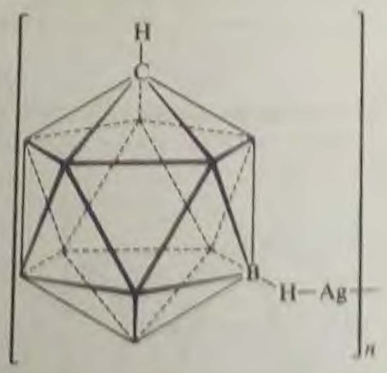
Todd, L.J. *et al, Inorg. Chem.*, 1970, **9**, 2175 (*synth*)

IC-002654

$CH_{12}AgB_{11}$

(Dodecahydro-1-carbadodecaborato)silver

[98194-47-9]



M 250.8

closo-. Clear colourless cryst. (C_6H_6). Sol. C_6H_6. When dry, air-stable in dark indefinitely. Ir ν_{BH} 2550 (mull); 2550, 2380 cm^{-1} (C_6H_6).

Bis-benzene adduct: [98194-48-0].

Transparent cryst. (C_6H_6/hexane). Cryst. slowly lose C_6H_6. Contains η^2-benzene to Ag bonding, with each Ag H-bonded to two borane units in a chain struct.

Shelly, K. *et al, J. Am. Chem. Soc.*, 1985, **107**, 5955 (*synth, cryst struct*)

IC-002655

$CH_{12}B_2N_2$

Methylhydrazine bis(borane)

Hexahydro[μ-(methylhydrazine-N:N′)]diboron, 10CI

Methylhydrazine compd. with borane(1:2), 9CI

[58978-79-3]

$H_3B—H_2NNHMe—BH_3$

M 73.7

Used in photographic image development.

Hamilton, J.F., *J. Vac. Sci. Technol.*, 1976, **13**, 319.

Gysling, H.J. *et al, Res. Discl.*, 1976, **142**, 34.

U.S. Pat., 4 042 392, (1977); *CA*, **88**, P30399w.

Ger. Pat., 2 819 885, (1978); *CA*, **90**, P178152x.

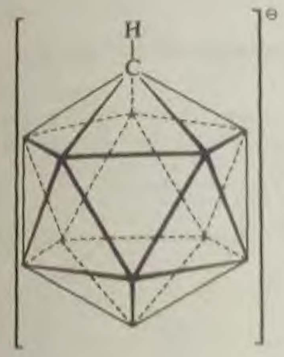
Lelental, M. *et al, J. Photogr. Sci.*, 1978, **26**, 135.

IC-002656

$CH_{12}B_{11}^{\ominus}$

Dodecahydro-1-carbadodecaborate(1−), 10CI, 9CI, 8CI

[73758-08-4]



M 143.0 (ion)

closo-.

Cs salt: [12539-26-3].

$CH_{12}B_{11}Cs$ M 275.9

Colourless solid. Sol. MeCN.

Me_4N salt: [92571-45-4].

Colourless solid. Sol. MeCN.

[38192-46-0]

Knoth, W.H. *et al, J. Am. Chem. Soc.*, 1967, **89**, 1274 (*synth, ir, B-11 nmr*)

Knoth, W.H. *et al, Inorg. Chem.*, 1971, **10**, 598 (*synth, ir, pmr, B-11 nmr*)

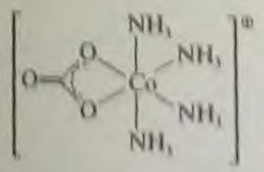
Wiersma, R.J. *et al, Inorg. Chem.*, 1973, **12**, 785 (*B-11 nmr, electrochem*)

IC-002657

$CH_{11}CoN_4O_3^{\oplus}$

Tetraammine[carbonato(2−)-*O,O′*]cobalt(*III*)(1+), 9CI

[23025-97-0]



M 187.0 (ion)

Classic example of bidentate $CO_3^{2\ominus}$.

Bromide: [14319-92-7].

Cryst.

Barclay, G.A. *et al, J. Chem. Soc.*, 1962, 586 (*synth, cryst struct*)

Snow, M.R. *et al, Aust. J. Chem.*, 1972, **25**, 1307 (*cryst struct*)

IC-002658

$CH_{12}CoN_5O_3S$

Tetraamminecyano(sulfito)cobalt(*III*)

$Co(NH_3)_4(SO_3)(CN)$

M 233.1

Stereochem. not determined, prob. monodentate $SO_3^{2\ominus}$.

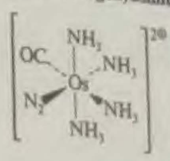
Orange cryst.

Sieber, H. *et al, Z. Anorg. Allg. Chem.*, 1964, **327**, 63 (*synth, ir*)

IC-002659

$CH_{12}N_6OOs^{2\oplus}$

Tetraamminecarbonyl(dinitrogen)osmium(*II*)(2+)



M 314.3 (ion)

Dichloride: [39176-88-0].

Synth. from $[Os(NH_3)_5CO]Cl_2$, KNO_2 and HCl. White solid. Ir ν_{NN} 2179s; ν_{CO} 1952vs cm^{-1}.

Dibromide: [39176-89-1].

Synth. as for iodide but using KBr. Ir $\nu_{N\equiv N}$ 2174; $\nu_{C\equiv O}$ 1956s cm^{-1}.

Diiodide: [39176-90-4]

Synth. from $[Os(NH_3)_5CO]Cl_2$, $NaNO_2$ and HCl followed by saturation with KI. Ir ν_{NN} 2189s; ν_{CO} 1975s cm^{-1}.

Allen, A.D. *et al, Can. J. Chem.*, 1972, **50**, 3093 (*synth, ir, ms*)

Buhr, J.D. *et al, Inorg. Chem.*, 1980, **19**, 2425 (*synth, ir*)

IC-002660

$CH_{12}N_6ORuS^{1\oplus}$

Tetraammine(nitrosyl)(thiocyanato-*N*)ruthenium(2+), 9CI

Tetraammine(isothiocyanato)(nitrosyl)ruthenium(2+)

[52581-62-1]

$[Ru(NO)(NCS)(NH_3)_4]^{2\oplus}$

M 257.2 (ion)

trans-Octahedral cation. Sol. H_2O.

Bis-thiocyanate: [54438-81-2].

Ir ν_{NO} 1886 cm^{-1}.

Sinitsyn, N.M. *et al, Koord. Khim.*, 1976, **2**, 1381 (*ir*)

IC-002661

$CH_{11}N_5O_3Ru^{1\oplus}$

Tetraammine(cyanato-*N*)(nitrosyl)ruthenium(2+)

$[Ru(NO)(NCO)(NH_3)_4]^{2\oplus}$

M 241.2 (ion)

trans-Octahedral cation. Prep. by treating Tetraamminechloro(nitrosyl)ruthenium(2+), IC-016436 in hot acidic soln. with KNCO. Sol. H_2O.

Diiodide: Orange salt. Ir ν_{NO} 1890 cm^{-1}.

Schreiner, A.F. *et al, Inorg. Chem.*, 1973, **11**, 880 (*synth, ir, ms, mcd*)

Inorg. Synth., 1976, **16**, 13 (*synth*)

CH_xB_yRe IC-002882

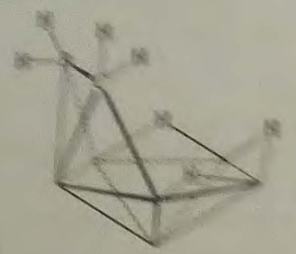
[Decahydrodiquadricosa(2+)-bis(hydrocyclium, 10C]

[65559-39-9]

M (R)
soln.- Air- and moisture-sensitive volatile liq. Unstable at −30°. Sol. C_6H_6, toluene
3-Pentylene and ions
Gunn, D.F. et al, Inorg. Chem., 1978, 17, 1358 (synth, s, R-C ass, ion, impt)

CH_xB_y IC-002883

6-Carbanonaborane(12)

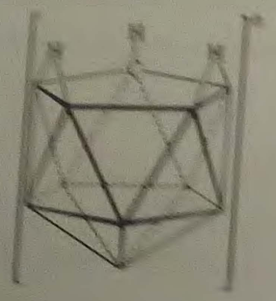


M 108.7
oxides- Moisture sensitive colourless solid. Sol. $CHCl_3$.
Pasek, J. et al, J. Chem. Soc., Chem. Commun., 1988, 568 (synth, ass, R-C ass, chir, str)

$CH_xB_y^{2-}$ IC-002884

Tridecahydro-7-carbanidecaborate(1−), bis(tricyclohexylphosphine)iminium, 10C2, 9C3, 8C1

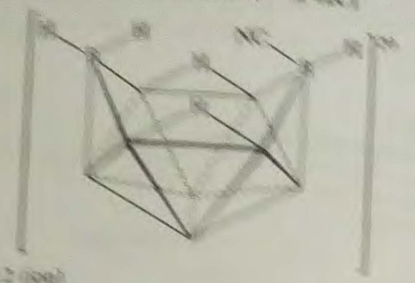
[52598-57-6]



M 135.2 (ion)
salts-
Cs salt: [12259-30-7]
CH_xB_yCs M 266.1
Air stable colourless solid. Sol. Me_2CO, H_2O; insol. DMF.
Me_4N salt: [12352-55-5]
Air stable colourless cryst. (MeOH/Me_2CO). Mod. sol. Me_2CO, DMF; insol. H_2O.
[51391-30-1]
Grant, D.E. et al, Inorg. Chem., 1967, 6, 2229 (synth, ir, pmr, R-C ass)
Inorg. Synth., 1968, 11, 39 (synth, ir, pmr)
Khan, S.A. et al, J. Chem. Soc., Dalton Trans., 1980, 2053 (electrochem)

$CH_xB_yV^{3+}$ IC-002885

6-Cyanotridecahydrodivanadecaborate(2−), 12C1

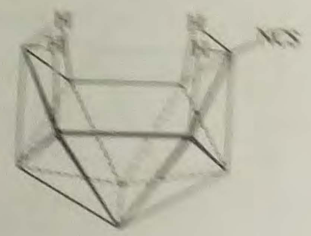


M 147.2 (ion)
oxides-
*Zn*Cl: salt: [51250-00-5]
Solid.
Bis-Me_2PhN salt: [12080-07-4]
Colourless cryst. (EtOH). Sol. H_2O.
Knoth, W.H. et al, J. Inorg. Nucl. Chem., 1967, 29, 91 (synth, str)
Bath, S. et al, Collect. Czech. Chem. Commun., 1981, 46, 2202 (synth)
Bath, S. et al, J. Chem. Soc., Chem. Commun., 1985, 341 (pmr, R-C ass, cryst struct)

CH_xB_yNS IC-002886

6-Dithiocyanatodecaborate(1+), 9C1, 8C1

[52680-23-8]

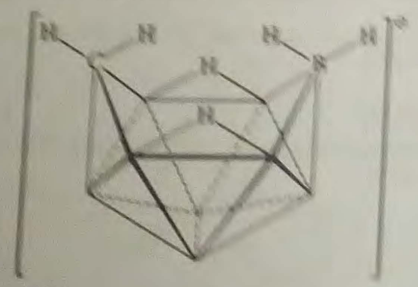


M 179.2
oxides-. Colourless cryst. (pentane). Sol. CS_2. Mp 84-85°.
Stibr, B. et al, Collect. Czech. Chem. Commun., 1971, 36, 1794 (synth, ir, R-C ass)
Hanousek, F. et al, Collect. Czech. Chem. Commun., 1972, 37, 3001 (synth, ir)
Kendall, D.S. et al, Inorg. Chem., 1973, 12, 2615 (cryst struct)

$CH_xB_y^{2-}$ IC-002887

Tetradecahydro-6-carbadecaborate(1−), 12C1

6-Carbadecaborate(14)(2−)



M 123.4 (ion)
oxides-
Cs salt: [115636-83-6]
Solid.
Me_4N salt: [115636-84-7]

Crystallogr. cryst. (Me_2CO sol.). Sol. $MeNO_2$. Mp 220-221°, subl. [11136-83-4]
[24387-95-0] (ClO4, solvated)
Sellmann, D. et al, J. Chem. Soc., Chem. Commun., 1987, 465 (synth, str, R-C ass, cryst)
Sellmann, D. et al, J. Chem. Soc., Dalton Trans., 1988, 2887 (synth, R-C ass)

$CH_xN_2O_2Re^{3+}$ IC-002888

Tetraaquadioxo(cyclam)rhenium(2+), 9C1

$[Re(NH_2)_4(OH)(OH_2)_2]^{3+}$

M 515.5 (ion)
halide-*chloride*
[60103-85-9]
sulfate [60103-85-9]
Prep. by reducing *cis*-bisammoniachlororhenium(III)(1+), IC-210000 with Zn/Hg, followed by CO.
perchlorate [36228-98-8]
$CH_xCl_3N_2O_2Re$ M 388.1
Yellow salt. Ir $\nu_{Re=O}$ 920 cm^{-1}
thiocyanate [33930-25-5]
$CH_xRe_2N_4O_4S_4$ M 575.0
Yellow salt. Ir $\nu_{Re=O}$ 930 cm^{-1}
iodide [36929-99-5]
$CH_xI_2N_2O_2Re$ M 469.0
Yellow salt. Ir $\nu_{Re=O}$ 1942 cm^{-1}
sulfate [60168-59-6]
hydroiodide [35501-16-8]
Prep. by passing CO through a slurry of chloride salt + bisammoniachlororhenium(III) dioxidorhenium(III)(1+), IC-210432 in HCOOH. Yellow salt. Ir $\nu_{Re=O}$ 1919 cm^{-1}
bromide [35501-17-9]
Yellow salt. Ir $\nu_{Re=O}$ 1924 cm^{-1}
iodide [35707-60-3]
Yellow salt. Ir $\nu_{Re=O}$ 1935 cm^{-1}
Lim, A.R. et al, Can. J. Chem., 1988, 47, 1805 (synth, s, str, reactions)
Hall, S.S. et al, Inorg. Chem., 1976, 15, 3030 (reactions)

$CH_xNa_2O_8$ IC-002889

Sodium carbonate (Na_2CO_3) heptahydrate

Carbonic acid, disodium salt, heptahydrate, 8C1

[5968-31-6]

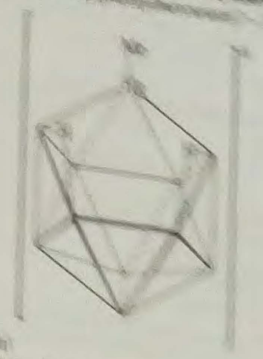
$Na_2CO_3 \cdot 7H_2O$

M 232.0
Colourless efflorescent orthorhombic cryst. V. sol. H_2O (54 g/100 cm^3 at 35°). ΔH_f° −3203.4 kJ mol^{-1}; ΔG_f° −2710.8 kJ mol^{-1}; S° 595.8 K^{-1} mol^{-1}
Sunr, T.W. et al, Can. J. Chem., 1952, 30, 76 (thermodyn data)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1961, 8, 1332 (rev, ref)
Bilz, K. et al, Spectrochim. Acta, 1963, 17, 917 (ir)
Dunstan, M.S. et al, Acta Crystallogr., 1963, 16, 555 (cryst struct)
Beni, C. et al, Acta Crystallogr., Sect. B, 1982, 38, 2662 (cryst struct)

$CH_xN_2O_2Re^+$

[(*Trans*)-Dioxobis(tetrahydroborato)(2−)-bis(ethylenediamine)(1−)-rhenium(V)]

IC-002975

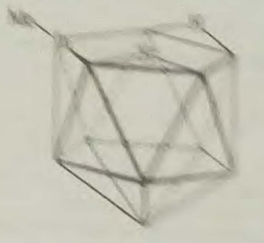


M 375.8 (ion)
Tentative struct. shown. Sol. CH_2Cl_2, $CHCl_3$, THF, Me_2CO; insol. hexane, H_2O.
Ko/Na-P salt: [39032-28-0]
Air-stable orange cryst. (CH_2Cl_2/Et_2O).
Greenwood, N.N. et al, J. Chem. Soc., Dalton Trans., 1972, 259 (synth, str, reactions)

$CH_xN_2O_2Re$

[(*Trans*)-Dioxobis(tetrahydroborato)(2−)-bis(ethylenediamine)(1−)-rhenium(V)]

IC-002976



M 250.0
Pale-yellow solid. Sol. Me_2CO.
Greenwood, N.N. et al, J. Chem. Soc., Dalton Trans., 1972, 259 (synth, s, reactions)

$CH_xCoF_3N_4O_4S^{2+}$ IC-002978

Pentaammine(trifluoromethanesulfonato-*O*)cobalt(III) (2+) x 1OC1

$[Co(NH_3)_5(OSO_2CF_3)]^{2+}$

M 293.1 (ion)
Octahedral with monodentate $CF_3SO_3^-$.
Bis-trifluoromethanesulfonate [33525-90-8]
$C_2H_{15}CoF_6N_4O_6S_2$ M 501.2
Violet cryst., stable for long periods in sealed container, dec. slowly on exp. to moisture. Sol. H_2O, F_3CSO_3H.
Dickson, N.E., Inorg. Chem., 1981, 20, 470 (synth, ir, kinetics, mech)
Inorg. Synth., 1983, 22, 106 (synth)

$CH_xCoN_4O_3^+$ IC-002979

Pentaamminecarbonatocobalt(III)(1+) x 1C1

$[Co(NH_3)_5(OCO_2)]^+$

M 204.0 (ion)
Octahedral with monodentate carbonate group.

Bromide: [21336-67-4].
Carmine-red cryst.
Inorg. Synth., 1953, **4**, 171 (*synth*)
Freeman, H.C. *et al*, *J. Chem. Soc.*, 1965, 3194 (*synth, cryst struct*)

IC-002674

$CH_{15}CoN_6O^{2\oplus}$

Pentaamminecyanatocobalt(*III*), 8Cl

[19998-52-8]

$[(H_3N)_5CoNCO]^{2\oplus}$

M 186.1 (ion)
Simple example of cyanate complex.
Diperchlorate: [27427-52-7].
Red cryst. solid.
▷ Potentially explosive.
Balaruha, R.J., *Inorg. Chem.*, 1970, **9**, 1567 (*synth, ir, pmr*)

IC-002675

$CH_{15}CoN_6Se^{2\oplus}$

Pentaammine(selenocyanato-*N*)cobalt(*III*)(2+), 9Cl

Pentammine(isoselenocyanato)cobalt(III)

$[Co(NH_3)_5NCSe]^{2\oplus}$

M 249.0 (ion)
Dibromide: [25729-97-9].
Light orange solid.
Duffy, N.V., *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 519 (*synth, ir, uv*)
Meipolder, J.B., *Inorg. Chim. Acta*, 1975, **15**, 91 (*synth, ir, uv*)

IC-002676

$CH_{15}CrF_3N_5O_3S^{2\oplus}$

Pentaammine(trifluoromethanesulfonato-*O*)chromium(*III*)(2+), 11Cl

[84254-60-4]

$[Cr(OSO_2CF_3)(NH_3)_5]^{2\oplus}$

M 286.2 (ion)
Octahedral cation. Starting material: trifluoromethanesulfonato ligand easily substituted to give other pentaammine derivs.
Bis-trifluoromethanesulfonate: [84254-61-5]. *Chromium*(III) *trifluoromethanesulfonate pentaammine*
$C_3H_{15}CrF_9N_5O_9S_3$ M 584.3
Synth. from $[CrCl(NH_3)_5]Cl_2$ and trifluoromethanesulfonic acid under N_2; then Et_2O added. Pink solid. Stable in sealed container.
Curtis, N.J. *et al*, *Aust. J. Chem.*, 1983, **36**, 1495.
Dixon, N.E. *et al*, *Inorg. Chem.*, 1984, **23**, 2940.
Curtis, N.J. *et al*, *Inorg. Chim. Acta*, 1985, **100**, 275 (*use*)
Curtis, N.J. *et al*, *Inorg. Chem.*, 1986, **25**, 484 (*aquation*)
Inorg. Synth., 1986, **24**, 250 (*synth*)

IC-002677

$CH_{15}CrN_6^{2\oplus}$

Pentaammine(cyano-C)chromium(*III*)(2+), 11Cl, 10Cl, 9Cl

[42213-67-2]

$[Cr(CN)(NH_3)_5]^{2\oplus}$

M 163.1 (ion)
Octahedral cation.
Dichloride: [72509-67-2].
Synth. from $[Cr(DMSO)(NH_3)_5](ClO_4)_3$ and NaCN in DMSO + LiCl/MeOH. Yellow solid.
Diperchlorate: [72509-66-1].
Obt. from the dichlorides and aq. $NaClO_4$. Yellow cryst. (aq. $NaClO_4$).

▷ Potentially explosive.
Riccieri, P. *et al*, *Inorg. Chem.*, 1980, **19**, 853, 3279 (*synth, uv, ir, kinetics, photochem*)
Lee, S.H. *et al*, *Inorg. Chem.*, 1985, **24**, 1531 (*photochem*)
Zinato, E. *et al*, *J. Phys. Chem.*, 1985, **89**, 839 (*photochem*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 786 (*rev*)

IC-002678

$CH_{15}CrN_6O^{2\oplus}$

Pentaammine(cyanato-*N*)chromium(*III*)(2+), 11Cl, 10Cl

[68092-87-5]

$[Cr(NCO)(NH_3)_5]^{2\oplus}$

M 179.1 (ion)
Octahedral. Hydrol. to $[Cr(NH_3)_6]^{3\oplus}$.
Dichloride: [72609-21-3].
Dinitrate: [68092-88-6].
Obt. by thermal dec. of molten $Cr(NO_3)_3 \cdot 10H_2O$/urea mixt. Bright orange cryst.
Schmidtke, H.-H. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **443**, 225 (*synth, ir, uv*)
Schoenherr, T. *et al*, *Inorg. Chem.*, 1979, **18**, 2726 (*ir, raman*)
Yang, D. *et al*, *Polyhedron*, 1983, **2**, 1267 (*hydrol*)

IC-002679

$CH_{15}CrN_6S^{2\oplus}$

Pentaammine(thiocyanato-*N*)chromium(*III*)(2+), 11Cl, 10Cl, 9Cl

[16884-60-9]

$[Cr(NCS)(NH_3)_5]^{2\oplus}$

M 195.2 (ion)
Octahedral.
Diperchlorate: [22478-28-0].
Synth. from the dinitrate and aq. $NaClO_4$. Orange solid (H_2O).
▷ Potentially explosive.
Dinitrate: [22478-27-9].
Synth. from $[Cr(OH_2)(NH_3)_5](NO_3)_3$ with $[NH_4]NCS$ in 0.01*M* HCl/MeOH. Yellow orange cryst. (0.01*M* HCl/$NaNO_3$).
Dithiocyanate: Chromium(III) *thiocyanate pentaammine*
$C_3H_{15}CrN_8S_3$ M 311.3
Synth. from $[CrCl(NH_3)_5]Cl_2$ or $[Cr(OH_2)(NH_3)_5](NO_3)_3$ and hot KCNS/HOAc. Orange solid.
Zinato, E. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 449; *J. Am. Chem. Soc.*, 1969, **91**, 1076 (*synth*)
Garner, C.S. *et al*, *Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Kirk, A.D. *et al*, *Inorg. Chim. Acta*, 1978, **27**, 265 (*synth, uv*)
Lee, S.H. *et al*, *Inorg. Chem.*, 1985, **24**, 1531 (*photochem*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 786 (*rev*)

IC-002680

$CH_{15}F_3IrN_5O_3S^{2\oplus}$

Pentaammine(trifluoromethanesulfonato)iridium(*III*), 11Cl

$[Ir(NH_3)_5(OSO_2CF_3)]^{2\oplus}$

M 426.4 (ion)
Trifluoromethanesulfonate: [84254-59-1].
White solid. Sol. H_2O.
Dixon, N.E. *et al*, *Inorg. Chem.*, 1984, **23**, 2940 (*synth, ir, uv, kinetics*)

IC-002681

$CH_{15}F_3N_5O_3OsS^{2\oplus}$

Pentaammine(trifluoromethanesulfonato-*O*)osmium(*III*)(2+), 11Cl

Pentaammine(triflato)osmium(III)(2+)

$[Os(NH_3)_5(OSO_2CF_3)]^{2\oplus}$

M 424.4 (ion)
Useful synthetic intermed.
Bis-trifluoromethylsulfonate: Osmium(III) *trifluoromethylsulfonate pentaammine*
$C_3H_{15}F_9N_5O_9OsS_3$ M 722.5
Synth. by dissolving $[Os(NH_3)_5N_2]Cl_2$ in CF_3SO_3H followed by oxidation with Br_2.
Lay, P.A. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 7658.
Harman, W.D. *et al*, *J. Am. Chem. Soc.*, 1990, **112**, 2261 (*use*)

IC-002682

$CH_{15}F_3N_5O_3PtS^{3\oplus}$

Pentaammine(trifluoromethanesulfonato-*O*)platinum(*IV*)(3+), 11Cl

Pentaammine(trifluoromethylsulfato)platinum(IV)(3+)

$[Pt(NH_3)_5(OSO_2CF_3)]^{3\oplus}$

M 429.3 (ion)
Octahedral struct. Synth. from Pentaammine(chloro) platinum(*IV*)(3+), IC-016444 + CF_3SO_3H. Useful for synth. of other $[Pt(NH_3)_5L]^{4\oplus}$ species.
Tristrifluoromethylsulfonate: [84254-63-7].
White solid. Sol. CF_3SO_3H.
Dixon, N.E. *et al*, *Inorg. Chem.*, 1983, **22**, 846; 1984, **23**, 2940 (*synth, ir, uv, pmr, reactions*)
Inorg. Synth., 1986, **24**, 277 (*synth*)

IC-002683

$CH_{15}F_3N_5O_3RhS^{2\oplus}$

Pentaammine(trifluoromethanesulfonato-*O*)rhodium(*III*)(2+), 11Cl

$[Rh(NH_3)_5(OSO_2CF_3)]^{2\oplus}$

M 337.1 (ion)
Octahedral complex.
Bis-trifluoromethanesulfonate: [84254-57-9]. *Rhodium*(III) *trifluoromethanesulfonate pentaammoniate*
Pale yellow solid.
Dixon, N.E. *et al*, *Inorg. Chem.*, 1984, **23**, 2940 (*synth, ir, uv, pmr*)

IC-002684

$CH_{15}IrN_5O_3^{\oplus}$

Pentaammine[carbonato(2−)-*O*]iridium(*III*)(1+), 9Cl

[50600-91-4]

$[Ir(NH_3)_5(CO_3)]^{\oplus}$

M 337.3 (ion)
Perchlorate: [50600-92-5].
White solid. Sol. H_2O.
▷ Potentially explosive.
Palmer, D.A. *et al*, *Inorg. Chem.*, 1974, **13**, 965 (*synth, kinetics*)
Inorg. Synth., 1977, **17**, 152 (*synth*)

IC-002685

$CH_{15}IrN_6S^{2\oplus}$

Pentaammine(thiocyanato-*N*)iridium(*III*)(2+), 9Cl

Pentammine(isothiocyanato)iridium(III)(2+)

$[Ir(NH_3)_5(NCS)]^{2\oplus}$

M 335.4 (ion)
Diperchlorate: [15691-81-3].
White cryst. Sol. H_2O, sl. sol. Me_2CO.
▷ Potentially explosive.
Schmidtke, H.H., *Inorg. Chem.*, 1966, **5**, 1682 (*synth, ir, uv-vis*)
Inorg. Synth., 1970, **12**, 243 (*synth*)
Wagner, F.E. *et al*, *Chem. Phys.*, 1974, **4**, 284 (*mössbauer*)

IC-002686

$CH_{15}IrN_6S^{2\oplus}$

Pentaammine(thiocyanato-*S*)iridium(*III*)(2+), 9Cl

[29589-10-4]

$[Ir(NH_3)_5(SCN)]^{2\oplus}$

M 335.4 (ion)
Linkage isomer of Pentaammine(thiocyanato-*N*) iridium(*III*)(2+), IC-002685.
Diperchlorate: White cryst.
▷ Potentially explosive.
Schmidtke, H.H., *Inorg. Chem.*, 1966, **5**, 1682 (*synth, ir, uv-vis*)
Flack, H.D. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 1099 (*cryst struct*)
Wagner, F.E. *et al*, *Chem. Phys.*, 1974, **4**, 284 (*mössbauer*).

IC-002687

$CH_{15}N_5OOs^{2\oplus}$

Pentaamminecarbonylosmium(*II*)(2+), 9Cl

[70528-08-4]

$[Os(NH_3)_5CO]^{2\oplus}$

M 303.3 (ion)
Dichloride: [39176-85-7].
Synth. by reaction of $[OsCl(NH_3)_5]Cl_2$ in formic acid with Zn and CO followed by addition of KCl.
Colourless powder. Ir ν_{CO} 1890, 1875, 1823; ν_{Os-C} 589; ν_{Os-NH_3} 450 cm^{-1}.
Dibromide: [39176-86-8].
Synth. analogous to chloride. Ir ν_{CO} 1895, 1883, 1830; ν_{Os-C}; ν_{Os-C} 561, ν_{Os-NH_3} 439 cm^{-1}.
Diiodide: [39176-87-9].
Synth. analogous to chloride. Ir ν_{CO} 1907, 1898, 1847; ν_{Os-C} 557; ν_{Os-NH_3} 433 cm^{-1}.
Allen, A.D. *et al*, *Can. J. Chem.*, 1972, **50**, 3093 (*synth*)
Buhr, J.D. *et al*, *Inorg. Chem.*, 1979, **18**, 2208; 1980, **19**, 2425 (*uv, ir, electrochem, uv*)
Harman, W.D. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 8223 (*use*)
Morris, R.H. *et al*, *Inorg. Chem.*, 1987, **26**, 2674 (*uv, pe*)

IC-002688

$CH_{15}N_5ORu^{2\oplus}$

Pentaammine(carbonyl)ruthenium(*II*)(2+), 9Cl

[31418-66-3]

$[Ru(NH_3)_5CO]^{2\oplus}$

M 214.2 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980-7 with CO or Aquacarbonyltetrachlororuthenate(2−), IC-002500 with aq. NH_3.
Dichloride: [23351-13-5].
$CH_{15}Cl_2N_5ORu$ M 285.1
Yellow salt. Ir ν_{CO} 1922 cm^{-1}.
Dibromide: [23351-14-6].
$CH_{15}Br_2N_5ORu$ M 374.0
Yellow salt. Ir ν_{CO} 1935 cm^{-1}.
Diiodide: [21884-94-6].
$CH_{15}I_2N_5ORu$ M 468.0
Yellow salt. Ir ν_{CO} 1948 cm^{-1}.
Bis-tetrafluoroborate: [34843-20-4].
Yellow salt. Ir ν_{CO} 1972 cm^{-1}.
Bis-hexafluorophosphate: [34843-19-1].
Yellow salt. Ir ν_{CO} 1994 cm^{-1}.
Campbell, C.H. *et al*, *J. Organomet. Chem.*, 1968, **14**, 349 (*synth, ir*)
Allen, A.D. *et al*, *Can. J. Chem.*, 1969, **47**, 1605 (*synth, reactions, uv*)
Stanko, J.A. *et al*, *Inorg. Chem.*, 1969, **8**, 2156 (*synth, ir, uv*)
Chatt, J. *et al*, *J. Chem. Soc. A*, 1971, 3168 (*synth, ir*)

Baranovski, V.I. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1973, **14**, 115 (*theory*)
Bee, M.W. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 585 (*ir, raman*)
Murrell, J.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1425 (*theory*)

IC-002689

$CH_{15}N_5O_3Rh^{\oplus}$

Pentaammine[carbonato(2−)-*O*]rhodium(*III*)(1+), 8CI

[50600-89-0]

$[RhCO_3(NH_3)_5]^{\oplus}$

M 248.0 (ion)
Perchlorate: [50600-90-3].
Pale yellow cryst. Sol. H_2O.
▷ Potentially explosive.

Palmer, D.A. *et al*, *Inorg. Chem.*, 1974, **13**, 965 (*synth, kinetics, uv*)
Spitzer, U. *et al*, *Inorg. Chem.*, 1982, **21**, 2821 (*kinetics, uv*)

IC-002690

$CH_{15}N_6ORh^{2\oplus}$

Pentaammine(cyanato-*N*)rhodium(2+), 8CI
Isocyanatopentamminerhodium(III)

$[Rh(NH_3)_5(NCO)]^{2\oplus}$

M 230.0 (ion)
Diperchlorate: [34420-30-9].
Pale yellow solid.
▷ Potentially explosive.

Ford, P.C. *et al*, *Inorg. Chem.*, 1971, **10**, 2153 (*synth, uv, kinetics*)

IC-002691

$CH_{15}N_6ORu^{2\oplus}$

Pentaammine(cyanato-*N*)ruthenium(*III*)(2+), 9CI

$[Ru(NH_3)_5(NCO)]^{2\oplus}$ (C_{4v})

M 228.2 (ion)
Prepd. by anation of $[Ru(NH_3)_5Cl]^{2\oplus}$ or oxidation of the ruthenium(*II*) analogue. Acid hydrol. yields $[Ru(NH_3)_6]^{3\oplus}$ and CO_2.
Diperchlorate: Yellow solid. Sol. H_2O.
▷ Potentially explosive.
Dibromide: [55101-90-1].
Yellow solid.

Ford, P.C., *Inorg. Chem.*, 1971, **10**, 2153 (*synth, hydrol*)
Lin, S.-W. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 290 (*synth, uv*)
Evans, R.S., *Inorg. Chem.*, 1975, **14**, 1705 (*mcd*)

IC-002692

$CH_{15}N_6RuS^{2\oplus}$

Pentaammine(thiocyanato-*N*)ruthenium(*III*)

$[Ru(NH_3)_5(NCS)]^{2\oplus}$ (C_{4v})

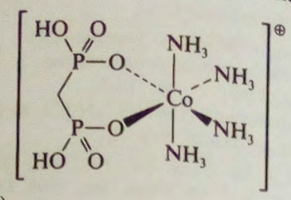
M 244.3 (ion)
Only the *N*-bonded thiocyanato isomer has been observed. Reports of the *S*-bonded isomer are unsupported.
Prepd. by oxidation of ruthenium(*II*) analogue.
Addition of $Hg^{2\oplus}$ to aq. soln. changes colour to yellow.
Diperchlorate: [38139-15-0].
Violet-red cryst. Sol. H_2O.
▷ Potentially explosive.

Lin, S.-W. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 290 (*purported S-bonded isomer*)
Lim, H.S. *et al*, *Inorg. Chem.*, 1972, **11**, 1460 (*synth, uv, electrochem*)

IC-002693

$CH_{16}CoN_4O_6P_2^{\oplus}$

Tetraammine(methylenediphosphato)cobalt(*III*)(1+)



M 301.0 (ion)
Octahedral coordination at Co. The methylenediphosphato ligand has the half chair conform.
Chloride: [90791-30-3].
Tetraammine[[methylenebis[phosphonato]](4−)] cobaltate(1−) hydrogen chloride (1:2:1), 11CI
Dark red cryst.

Haromy, T.P. *et al*, *Inorg. Chem.*, 1984, **23**, 2412 (*synth, cryst struct*)

IC-002694

$CH_{16}CoN_5O_2^{2\oplus}$

Pentaammine(formato-*O*)cobalt(*III*)(2+), 9CI

[19173-64-9]

$[(H_3N)_5Co(OOCH)]^{2\oplus}$

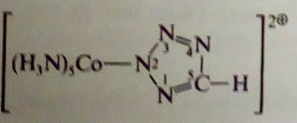
M 189.1 (ion)
Diperchlorate: [28660-81-3].
Sol. H_2O.
▷ Potentially explosive.
Dinitrate: [52524-46-6].
Sol. DMSO.

Barrett, M. *et al*, *Inorg. Chem.*, 1971, **9**, 1983 (*synth, kinetics*)
Balahura, R.J. *et al*, *Inorg. Chem.*, 1973, **12**, 1438 (*synth*)
Yoshida, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 669 (*synth, pmr*)

IC-002695

$CH_{16}CoN_9^{2\oplus}$

Pentaammine(1*H*-tetrazolato-N^2)cobalt(*III*)(2+), 11Cl



M 213.1 (ion)
Bis-tetrafluoroborate: [87371-43-5].
5-Cyano, bis-tetrafluoroborate: [87371-39-9].
Pentaamine(1H-tetrazole-5-carbonitrilato-N^2)cobalt(III) (2+) *tetrafluoroborate*
5-Me: see *Pentaammine(5-methyl-1H-tetrazolato)cobalt*(III) (2+), *IC-003393*
5-Ph: see *Pentaammine(5-phenyl-1H-tetrazolato)cobalt*(III) (2+), *IC-005812*
5-Carboxamide: see *Pentaammine(1H-tetrazole-5-carboxamidato-N^1)cobalt*(III)(2+), *IC-003384*

Graeber, E.J. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 567 (*cryst struct*)
Balahura, R.J. *et al*, *Inorg. Chem.*, 1983, **22**, 3602 (*synth, pmr, cmr, N-15 nmr, uv, redox kinetics, deriv*)

IC-002696

$CH_{16}IrN_5O_2^{2\oplus}$

Pentaammineformatoiridium(*III*)(2+), 9CI

[52795-08-1]

$[Ir(NH_3)_5(OOCH)]^{2\oplus}$

M 322.3 (ion)
Diperchlorate: [15646-83-0].

White cryst.
Schmidtke, H.H., *Inorg. Chem.*, 1966, **5**, 1682 (*synth*)
Wagner, F.E. *et al*, *Chem. Phys.*, 1974, **4**, 284 (*mössbauer*)
Curtis, N.J. *et al*, *Aust. J. Chem.*, 1983, **36**, 1327 (*electrochem*)

IC-002697

$CH_{16}N_5O_2Rh^{2\oplus}$

Pentaammineformatorhodium(*III*)(2+), 8CI

$[Rh(NH_3)_5(OOCH)]^{2\oplus}$

M 233.0 (ion)
Diperchlorate: [15612-60-9].
White cryst. Sol. H_2O.
▷ Potentially explosive.

Schmidtke, H.H. *et al*, *Z. Phys. Chem. (Frankfurt am Main)*, 1965, **45**, 305 (*synth*)
Monacelli, F. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1079 (*synth, kinetics*)

IC-002698

$CH_{16}N_5O_2Ru^{\oplus}$

Pentaammine(formato)ruthenium(*II*)(1+), 9CI
Pentaammine(methanoato)ruthenium(II)(1+)

$[Ru(NH_3)_5OOCH]^{\oplus}$

M 231.2 (ion)
Undergoes rapid aquation (k_{aq} 1.28 s^{-1}). Prepd. by electrochemical reduction of Pentaammine(formato-*O*) ruthenium(*III*)(2+), IC-002699. Only obsd. in soln. Sol. H_2O.

Stritar, J.A. *et al*, *Inorg. Chem.*, 1969, **8**, 2281 (*synth, electrochem, uv, aquation*)

IC-002699

$CH_{16}N_5O_2Ru^{2\oplus}$

Pentaammine(formato-*O*)ruthenium(*III*)(2+), 9CI
Pentaamminemethanoatoruthenium(III)(2+)
[38744-90-0]

$[Ru(NH_3)_5(O_2CH)]^{2\oplus}$

M 231.2 (ion)
Prepd. by oxidising the ruthenium(*II*) analogue. Readily reduced by common one-electron reducing reagents; undergoes a wide range of anation and aquation reaction.
Diperchlorate: Yellow solid. Sol. H_2O.
▷ Potentially explosive.

Stritar, J.A. *et al*, *Inorg. Chem.*, 1969, **8**, 2281 (*synth, uv, reactions*)
Lin, S.-W. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 290 (*uv*)
Ohyoshi, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2121; 1973, **46**, 2431 (*reactions*)
Ohkubo, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 2651; 1975, **48**, 774 (*reactions*)
Ohyoshi, A. *et al*, *Chem. Lett.*, 1973, 737 (*electrochem*)

IC-002700

$CH_{17}CoN_6O_2^{2\oplus}$

Pentaammine(carbamato-*O*)cobalt(*III*)(2+), 9CI

[19173-65-0]

$[Co[OC(O)NH_2](NH_3)_5]^{2\oplus}$

M 204.1 (ion)
Diperchlorate: Sol. H_2O.

Sargeson, A.M. *et al*, *Inorg. Chem.*, 1966, **5**, 1094 (*synth, uv*)
Buckingham, D.A. *et al*, *Inorg. Chem.*, 1974, **13**, 2630 (*ir, uv*)

IC-002701

$CH_{17}CoN_7^{3\oplus}$

Pentaammine(cyanamide)cobalt(*III*)(3+), 8CI

[31303-35-2]

$[Co(N{\equiv}CNH_2)(NH_3)_5]^{3\oplus}$

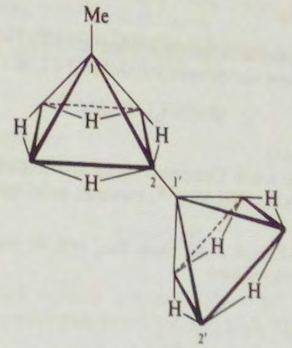
M 186.1 (ion)
Octahedral geometry presumed. Kinetics of the chromium(*II*) reduction for this complex have been studied.
Triperchlorate: Not isol. Sol. H_2O, DMSO.
▷ Potentially explosive.

Balahura, R.J. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 625 (*synth, uv, pmr, props, kinetics*)

IC-002702

$CH_{18}B_{10}$

2-(1′-Pentaboran-9-yl)-1-methylpentaborane(9)
Di-1-pentaborylmethane
[89017-48-1]



M 138.2
conjuncto-. Synth. by cophotolysis of a 70% B_5H_9/30% 1-MeB_5H_8 mixt.

Sneddon, L.G. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 2275 (*synth, B-11 nmr*)

IC-002703

$CH_{18}CoN_5O_3S^{2\oplus}$

Pentaammine(methanesulfonato-*O*)cobalt(*III*)(2+), 10CI

$[Co[OS(O)_2Me](NH_3)_5]^{2\oplus}$

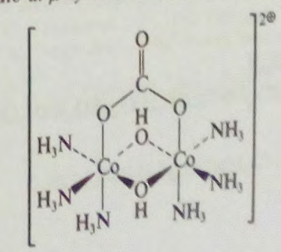
M 239.1 (ion)
Diperchlorate: [76024-71-0].
Pink solid. Sol. DMSO.

Buckingham, D.A. *et al*, *Inorg. Chem.*, 1981, **20**, 1647 (*synth, uv, pmr, kinetics*)

IC-002704

$CH_{20}Co_2N_6O_5^{2\oplus}$

Hexaammine[μ-[carbonato(2−)-*O*:*O*′]]di-μ-hydroxydicobalt(2+), 10CI
μ-Carbonato-di-μ-hydroxo-bis[triamminecobalt(III)]



M 314.0 (ion)
Bioctahedral cation.

Sulfate: [75476-69-6].
Red cryst. + $5H_2O$. Sol. H_2O; insol. non-aq. solvs.

Churchill, M.R. *et al, Inorg. Chem.*, 1981, **20**, 376 (*synth, cryst struct*)

IC-002705

$CH_{20}N_6Ru^{2\oplus}$

Pentaammine(methylamine)ruthenium(*II*)(2+)
Pentaammine(methanamine)ruthenium(2+)

$[(H_3N)_3RuNH_2Me]^{2\oplus}$

M 217.2 (ion)
Sol. dil. HCl.
Bis-hexafluorophosphate: [56082-86-1].
Synth. from Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 + methylamine, followed by $[NH_4][PF_6]$. Yellow cryst.

Diamond, S.E. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2661 (*synth, electrochem, oxidation*)

IC-002706

$CH_{20}N_6Ru^{3\oplus}$

Pentaammine(methylamine)ruthenium(*III*)(3+)
Pentaammine(methanamine)ruthenium(3+), 9Cl

$[Ru(NH_3)_5NH_2Me]^{3\oplus}$

M 217.2 (ion)
Not isol. as a salt. Generated by electrochemical oxidation of $[Ru(NH_3)_5(NH_2Me)]^{2\oplus}$. Unstable soln. species. Sol. dil. HCl.

Diamond, S.E. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2661 (*synth, electrochem, reaction*)

IC-002707

$CH_{20}Na_2O_{13}$

Sodium carbonate (Na_2CO_3) decahydrate
Carbonic acid, disodium salt, decahydrate, 8CI. Washing soda
[6132-02-1]

$Na_2CO_3.10H_2O$

M 286.1
Synth. by cryst. from aq. Na_2CO_3. Heat storage material. Commercially available. White efflorescent monoclinic cryst. Dec. on heating by H_2O loss giving the monohydrate and the anhydrous material. V. sol. H_2O (22 g per 100 cm^3 at 0°; 421 g per 100 cm^3 at 104°); insol. EtOH. ΔH_f° −4082.5 kJ mol^{-1}; ΔG_f° −3424.3 kJ mol^{-1}; S° 53.6 J K^{-1} mol^{-1}.

Bauer, T.W. *et al, Can. J. Chem.*, 1952, **30**, 76 (*thermodyn data*)
Buijs, K., *Spectrochim. Acta*, 1961, **17**, 917 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 308; 1966, **3**, 1331 (*rev, bibl*)
Rinne, M. *et al, Bull. Soc. R. Sci. Liege*, 1967, **36**, 328; *CA*, 1968, **68**, 110101 (*Na-23 nmr*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1969, **18**, 458 (*rev, uses*)
Groenvold, F. *et al, J. Chem. Thermodyn.*, 1983, **15**, 881 (*cryst struct*)

IC-002708

$CH_{24}Ca_3MnO_{25}S$

Jouravskite ($Ca_3Mn^{IV}(OH)_6(CO_3)(SO_4)12H_2O$)
[12179-77-0]

$Ca_3Mn(OH)_6(CO_3)(SO_4).12H_2O$

M 643.4
Contains the Mn(*IV*) species $[Mn(OH)_6]^{2\ominus}$; Mn—OH 187 pm. Occurs in a dark mass of Mn minerals intimately associated with calcite, Morocco. Yellow-green to green-orange tiny embedded grains.

Granger, M.M. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 1943
Roberts, W.M. *et al, Encyclopedia of Minerals*, 2nd Ed., van Nostrand, N.Y., 1990, 420 (*rev, bibl*)

IC-002709

$CH_{24}Mg_6Mn_2O_{23}$

Desautelsite
[70212-18-9]

$Mg_6Mn_2(OH)_{16}CO_3.4H_2O$

M 659.8
Trivalent Mn analogue of Pyroaurite. Mineral, occurs at sites in USA and Japan. Bright orange cryst. Readily sol. aq. HCl. Hexagonal struct. Mg and Mn may be ordered.

Dunn, P.J. *et al, Am. Mineral.*, 1979, **64**, 127 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 218 (*rev, bibl*)

IC-002710

$CH_{30}Ca_3O_{25}SSi$

Thaumacite
[12539-13-8]

$Ca_3[Si(OH)_6][SO_4][CO_3].12H_2O$

M 622.6
Member of ettringite group. Hexahydroxo silicate. Mineral. Colourless or white cryst.

Kirov, G.N. *et al, Mineral. Mag.*, 1968, **36**, 1003 (*ir*)
Edge, R.A. *et al, Acta Crystallogr., Sect. B*, 1971, **27**, 594 (*cryst struct*)
Grimmer, A.R. *et al, Z. Chem.*, 1980, **20**, 453 (*solid state Si-29 nmr*)
Effenberger, H. *et al, Neues Jahrb. Mineral., Monatsh.*, 1983, 60 (*cryst struct*)

IC-002711

CHf

Hafnium carbide (HfC), 11CI
[12069-85-1]

HfC

M 190.5
NaCl struct. Several other phases have been reported in the Hf-C system but this is the only one which has been widely studied. Synth. by heating HfO_2 and C at 1700° or by melting above 2800°. Mp 3890°.

[11129-37-6]

Cotter, P.G. *et al, J. Am. Ceram. Soc.*, 1954, **37**, 415 (*synth, cryst struct*)
Curtis, C.E. *et al, J. Am. Ceram. Soc.*, 1954, **37**, 458 (*synth, cryst struct*)
Achour, M. *et al, Rev. Int. Hautes Temp. Refract.*, 1975, **12**, 289 (*synth*)

IC-002712

CHfN

Hafnium carbide nitride (HfCN), 11CI
[12601-88-6]

HfCN

M 204.5
Synth. by heating $HfCl_4$ with NH_3 and CH_2Cl_2 at 800°. Used in cermets and in coatings for cutting tools and gas turbine blades.

[58926-03-9]
Japan. Pat., 59 16 968, (1984); *CA*, **100**, 214501w (*synth*)
Ger. Pat., 2 043 411, (1971); *CA*, **75**, 24552f (*synth*)
Brundiers, G.D., *CA*, 1975, **85**, 9605p (*synth, props*)

IC-002713

CHfO

Hafnium carbide oxide (HfCO), 11CI
[101613-84-7]

HfCO

M 206.5
Composition is v. variable. Has defect NaCl struct. Synth. by heating HfO_2 and C to 2200°.

[57307-58-7]

Fedyukov, A.S. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1984, **20**, 1654; *CA*, **102**, 70606a (*cryst struct, high press, temp*)
Brundiers, G.D., *CA*, 1975, **85**, 9605p (*rev*)
Tverev, G.L., *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1197; *CA*, **69**, 73566y (*synth*)

IC-002714

$CHgN_2O_3$

Mercury cyanide nitrate ($Hg(CN)NO_3$)
[74227-08-6]

$Hg(NO_3)CN$

M 288.6
Contains infinite chains of (—Hg—CN—). Hg has additional contacts with 6 O from 3 NO_3 groups. Obt. by evap. of conc. soln. of $Hg(CN)_2$ and conc. HNO_3. Hexagonal cryst.

Mahon, C. *et al, Inorg. Chem.*, 1971, **10**, 2331 (*synth, ir, cryst struct*)

IC-002715

CHg_2O_3

Mercury(*I*) carbonate (Hg_2CO_3)
Carbonic acid, dimercury(1+) (1:1) salt
[6824-78-8]

Hg_2CO_3

M 461.1
Synth. from $Hg_2(NO_3)_2$ and K_2CO_3. White photosensitive powder, which dec. at 130°. Prac. insol. H_2O (4.5×10^{-4} g per 100 cm^3). Dec. by hot H_2O. Turns yellow on standing due to hydrol. K_{sp} 3.6×10^{-17} at 25°.

[13370-71-3]

Stammreich, H. *et al, J. Mol. Struct.*, 1967, **1**, 55 (*raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1186.

IC-002716

[CHo]

Holmium carbides

Known phases include Ho_3C, Ho_2C_3, HoC_2.

Holmium carbide (*HoC*$_2$) [12071-14-6]
C_2Ho M 188.9
Possesses CaC_2 struct. Brassy yellow solid. On hydrol., affords principally C_2H_2 but with some C_2H_4 and C_2H_6 and other hydrocarbons. Undergoes $\alpha \rightarrow \beta$ transition at 1305° (1280°). $\mu_{eff} = 10.47\mu_B$ (θ −25.6°).

Spedding, F.H. *et al, J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al, J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, magnetism*)
Misji, M., *J. Chem. Phys.*, 1967, **46**, 1891 (*magnetism*)

Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Sakai, T. *et al, J. Less-Common Met.*, 1981, **81**, 91 (*magnetism*)
Jones, D.W. *et al, J. Solid State Chem.*, 1984, **53**, 376 (*struct*)

IC-002717

CIN

Cyanogen iodide
Iodine cyanide

$IC{\equiv}N$ ($C_{\infty v}$)

M 152.9
Interatomic distances: I—C 199.4, C—N 115.9 pm. Synth. from NaCN + I_2. Used for destroying lower life forms; for preserving insects in taxidermy. Colourless needles ($CHCl_3$). Subl. Strong odour. Sl. sol. cold H_2O, sol. hot H_2O, EtOH. Mp 146.5°.
▷ V. poisonous.

Tyler, J.K. *et al, Trans. Faraday Soc.*, 1963, **59**, 2661 (*struct*)
Simpson, J.B. *et al, J. Mol. Spectrosc.*, 1972, **44**, 558 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 633 (*synth*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 988.

IC-002718

CINO

Iodine isocyanate
Iodoisocyanate
[3607-48-5]

$I{-}N{=}C{=}O$

M 168.9
Formed from $AgNCO + I_2$ in Et_2O at −20°. Photosensitive pale-brown oil. Sol. Et_2O, THF. Dec. at −11°.
▷ Explosive.

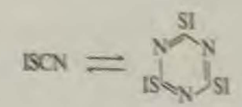
Trimer: see *1,3,5-Triiodo-1,3,5-triazine-2,4,6-trione*, IC-003766

Rosen, S. *et al, Anal. Chem.*, 1966, **38**, 1392 (*synth, ir*)
Gebelein, C.S. *et al, J. Org. Chem.*, 1968, **33**, 2758 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 143 (*bibl*)

IC-002719

CINS

Iodine thiocyanate, 9CI
[2010-58-4]



M 184.9
Adds to cyclic alkenes, providing a route to episulfides.

Trimer:
$C_3I_3N_3S_3$ M 554.9
Solid.

Nelson, M.J. *et al, J. Chem. Soc.*, 1960, 604 (*ir*)
Hinshaw, J.C., *Tetrahedron Lett.*, 1972, 3567 (*use*)
Raby, C. *et al, Comptes Rend. Hebd. Seances Acad. Sci. Ser. C*, 1976, **282**, 345.
Cambie, R.C. *et al, J. Chem. Soc., Perkin Trans. 1*, 1979, 757 (*synth, use*)

[ClORu] IC-002720

(Carbonyl)iodoruthenium(*I*)

$[Ru(CO)_2I]_n$

Struct. and formulation uncertain: prob. polymeric. Prepd. by treating $Ru(CO)_5$ with I_2, RuI_3 with CO, or Dicarbonyltetraiodoruthenate(2−), IC-003444 with CO. Orange solid. Sol. C_6H_6.

Manchot, W. *et al*, *Z. Anorg. Allg. Chem.*, 1936, **226**, 385 (*synth*)

$Cl_3OPd^{\ominus}$ IC-002721

Carbonyltriiodopalladate(1−)

[106816-63-1]

$[PdI_3(CO)]^{\ominus}$ (C_{2v})

M 515.1 (ion)

Catalyst/intermed. in reductive carbonylation of esters to aldehydes.

Tetrabutylammonium salt:
$C_{17}H_{36}I_3NOPd$ M 757.6
Readily loses CO in soln.

Graff, J.L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 337 (*use*)
Andreini, B.P. *et al*, *J. Organomet. Chem.*, 1988, **354**, 369 (*synth, ir*)

$Cl_3OPt^{\ominus}$ IC-002722

Carbonyltriiodoplatinate(1−)

[66213-26-1]

$[Pt(CO)I_3]^{\ominus}$

M 603.8 (ion)
Ir ν_{CO} 2078 cm^{-1} (CH_2Cl).
K salt: Red cryst. Mp 100° dec.
Tetrabutylammonium salt: [66213-27-2].
Orange cryst. (Me_2CO/Et_2O). Mp 128°.

Malatesta, L. *et al*, *Gazz. Chim. Ital.*, 1960, **90**, 1505 (*synth*)
Browning, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, raman, nmr*)
Andreini, B.P. *et al*, *J. Organomet. Chem.*, 1988, **354**, 357 (*ir*)

Cl_3ORh IC-002723

Carbonyltriiodorhodium, 8CI

Triiodocarbonylrhodium

[27857-60-9]

RhI_3CO

M 511.6
Black cryst. Ir ν_{CO} 2073 cm^{-1} (KBr).

Colton, R. *et al*, *Aust. J. Chem.*, 1970, **23**, 1351 (*synth, ir*)

Cl_3ORu IC-002724

Carbonyltriiodoruthenium(*III*), 8CI

[32073-82-8]

$Ru(CO)I_3$

M 509.7

Tentative identity of soln. species; it refers to the presence of a likely reactive moiety, rather than a specific species. Synth. (MeOH soln.) by exposing a suspension of RuI_3 in MeOH to CO (1atm.) for 1 week. Deep-red. Characterised spectroscopically. Sol. MeOH. Ir ν_{CO} 1995 cm^{-1} (MeOH).

Colton, R. *et al*, *Aust. J. Chem.*, 1969, **22**, 2011; 1971, **24**, 903 (*ir, synth*)

$Cl_5IrO^{2\ominus}$ IC-002725

Carbonylpentaiodoiridate(2−), 9CI

$[Ir(CO)I_5]^{2\ominus}$

M 854.7 (ion)

Di-K salt: [53728-64-6].
Cl_5IrK_2O M 932.9
Dark-red cryst.

Di-Cs salt: [30192-03-1].
CCs_2I_5IrO M 1120.5
No phys. props reported.

Bis-Et_4N salt: [28491-15-8].
Ir ν_{CO} 2019 cm^{-1} ($MeNO_2$).

Malatesta, L. *et al*, *J. Chem. Soc.*, 1964, 961 (*synth*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1970, 2788 (*synth, raman*)
Forster, D. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 221 (*synth, ir*)
Cleare, M.J. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 2019 (*ir, raman*)

$Cl_5ORh^{2\ominus}$ IC-002726

Carbonylpentaiodorhodate(2−), 10CI

Pentaiodocarbonylrhodate(2−)

[38840-34-5]

$[RhI_5CO]^{2\ominus}$ (C_{4v})

M 765.4 (ion)

Di-Cs salt: [29201-07-8].
CCs_2I_5ORh M 1031.2
Black cryst. Ir ν_{CO} 2020vs cm^{-1} (nujol).

Bis-Et_4N salt: Black cryst. Extremely insol. all solvs. Ir ν_{CO} 2040 cm^{-1} (nujol).

Forster, D., *Inorg. Chem.*, 1969, **8**, 2556 (*synth, ir*)
Colton, R. *et al*, *Aust. J. Chem.*, 1970, **23**, 1351 (*synth, ir*)
Dahm, D.J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 15 (*struct*)
Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1970, 2788 (*synth, ir, raman*)
Cleare, M.J. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 2019 (*raman, ir*)

$Cl_{14}Zr_6$ IC-002727

Dodeca-μ-iododiiodo-μ_6-methanetetraylhexazirconium, 11CI

Zirconium carbide iodide (Zr_6CI_{14}). Carbidododeca-μ-iododiiodohexazirconium

[98193-82-9]

As Dodeca-μ-chlorodichloro-μ_6-methanetetraylhexazirconium, IC-002381 with

X = I

M 2336.0
Synth. by heating ZrI_4, Zr and graphite in a sealed Ta tube at 850°. $Zr_6I_{12}C$ and $MZr_6I_{14}C$ (M = K, Rb, Cs) are also known.

Smith, J.D. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 5704 (*synth, cryst struct*)

CKN IC-002728

Potassium cyanide

[151-50-8]

KCN

M 65.1
NaCl struct. Synth. by neutralisation of KOH or K_2CO_3 with aq. HCN. Commercially available. Used in electroplating gold and silver. Also used to generate org. cyanides by reaction with the corresp. halides (cyanation reactions). Deliquescent colourless cubic cryst. Undergoes cubic to orthorhombic transition at −60°. V. sol. H_2O (72 g per 100 cm^3 at 25°); spar. sol. EtOH (0.88 g per 100 cm^3 at 20°); sol. MeOH (4.9 g per 100 cm^3 at 20°). Mp 622°. ΔH_f° −113.5 kJ mol^{-1}; ΔG_f° −102.0 kJ mol^{-1}; S° 128 J K^{-1} mol^{-1}.

▷ Highly toxic, irritant. TS8750000.

Bijvoet, J.M. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1940, **59**, 908 (*cryst struct*)
Gallais, F., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1942, **214**, 552 (*ir*)
Miller, F.A. *et al*, *Anal. Chem.*, 1952, **24**, 1253 (*ir*)
Pistorius, C.W. *et al*, *J. Chem. Phys.*, 1968, **48**, 5123 (*polymorphs*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 602 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2898B (*haz*)

CKNO IC-002729

Potassium cyanate

Cyanic acid, potassium salt, 8CI

[590-28-3]

K[OCN]

M 81.1
Struct. related to KHF_2. Synth. either by precipitation reaction of $Hg(OCN)_2$ + KSCN in Me_2CO or by mild oxidation of aq. KCN using Pb(*IV*). Commercially available. Used for the carbonitridation of steels. Colourless tetragonal cryst. V. sol. H_2O (75 g per 100 cm^3 at 25°); insol. EtOH. Dec. on heating → KCN + O_2.

▷ GS6825000.

Cleveland, F.F., *J. Am. Chem. Soc.*, 1941, **63**, 622 (*raman*)
Swanson, H.E. *et al*, *Natl. Bur. Std. Circ. (U.S.)*, 1957, **7**, 39 (*cryst struct*)
Beck, W., *Chem. Ber.*, 1962, **95**, 341 (*ir*)
Soderback, E., *Acta Chem. Scand.*, 1971, **25**, 3534 (*synth*)
Bloor, E.G. *et al*, *Can. J. Chem.*, 1972, **50**, 3926 (*K-39 nmr*)
Kanamori, K. *et al*, *Biochemistry*, 1983, **22**, 2658 (*N-15 nmr*)

$CKNO_4S_2Sn$ IC-002730

Potassium tin sulfate thiocyanate ($KSn(SO_4)(NCS)$)

Potassium (isothiocyanato)sulfatostannate(1−), 8CI

$KSn(SO_4)NCS$

M 311.9
Synth. from $SnSO_4$ + KNCS. Cryst.

Chamberlain, B.R. *et al*, *J. Chem. Soc. A*, 1969, 354 (*synth, ir, cryst struct*)

CKNS IC-002731

Potassium thiocyanate

Thiocyanic acid, potassium salt, 8CI

[333-20-0]

K[SCN]

M 97.1
Prepd. by fusing together KCN and sulfur. Commercially available. Used in electroplating solns., particularly for silver, and also for photographic developers. Colourless orthorhombic deliquescent. cryst. Undergoes orthorhombic to tetragonal transition at 160°. V. sol. H_2O (177 g per 100 cm^3 at 0°; 217 g per 100 cm^3 at 20°), Me_2CO (21 g per 100 cm^3 at 22°); sol. EtOH. Mp 173°. ΔH_f° −200 kJ mol^{-1}; ΔG_f° −178 kJ mol^{-1}; S° 124 J K^{-1} mol^{-1}.

▷ Toxic. Reaction with $KHSO_4$ yields free HNCS. XL1925000.

Klug, H.P., *Z. Kristallogr.*, 1933, **85**, 214 (*cryst struct*)
Tramer, A., *J. Chem. Phys.*, 1962, **59**, 232 (*ir, raman*)
Yamada, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1963, **36**, 1032 (*polymorphs*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 954.
Kargol, J.A. *et al*, *Inorg. Chim. Acta*, 1977, **25**, L109 (*cmr*)
Schmidt, E. *et al*, *Spectrosc. Lett.*, 1981, **14**, 787 (*K-39 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2911C (*haz*)

CKNSe IC-002732

Potassium selenocyanate

Selenocyanic acid, potassium salt, 8CI

[3425-46-5]

K[SeCN]

M 144.0
Synth. by melting together KCN + Se. Commercially available. Reagent for stereoselective conversion of epoxides to alkenes. Aq. solns. used in the synth. of insol. salts [MSeCN (M = Ag, Cu, Tl) or $M(SeCN)_2$ (M = Hg_2, Hg, Pb)]. Colourless monoclinic cryst.; deliquescent. Sol. H_2O, EtOH. Dec. on standing in air or on being heated above 100°.

▷ Highly toxic. VT1400000.

Inorg. Synth., 1946, **2**, 186 (*synth*)
Morgan, H.W., *J. Inorg. Nucl. Chem.*, 1961, **16**, 367 (*ir*)
Swank, D.D. *et al*, *Inorg. Chem.*, 1965, **4**, 499 (*cryst struct*)
Pan, W.H. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 5783 (*Se-77 nmr*)
Clive, D.L., *Tetrahedron*, 1978, **34**, 1049 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2909A (*haz*)

CK_2O_3 IC-002733

Potassium carbonate (K_2CO_3)

Carbonic acid, dipotassium salt, 8CI. Pearl ash

[584-08-7]

K_2CO_3

M 138.2
Synth. by reaction of CO_2 with KOH dissolved in MeOH or EtOH, or by thermal dehydration of the sesquihydrate. Commercially available. Catalyst for coal gasification. Also used in photographic developers, fire extinguishers and the production of speciality glasses and ceramics. Hygroscopic colourless monoclinic cryst. Undergoes polymorphic change at 250°. Dec. on heating with CO_2 loss. V. sol. H_2O (112 g per 100 cm^3 at 20°; 156 g per 100 cm^3); insol. EtOH, Me_2CO. Mp 901°. ΔH_f° −1150 kJ mol^{-1}; ΔG_f° −1065 kJ mol^{-1}; S° 155.5 J K^{-1} mol^{-1}.

▷ Irritant. TS7750000.

Sesquihydrate: [6381-79-9].
$C_2H_6K_4O_9$ M 330.4

Cryst. from aq. solns. of K_2CO_3 at 40°. Commercially available. Colourless monoclinic cryst. Dec. on heating with H_2O loss ($-\frac{1}{2}$ H_2O at 235°; $-1\frac{1}{2}$ H_2O at 273°). V. sol. H_2O (268 g per 100 cm^3 at 100°); insol. EtOH.

▷ Irritant.

Duval, C. *et al*, *Anal. Chem.*, 1959, **20**, 20 (*ir*)
Caranoni, C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **270**, 1106 (*hydrate, struct*)
Bloor, E.G. *et al*, *Can. J. Chem.*, 1972, **50**, 3926 (*K-39 nmr*)
Gatehouse, B.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 70 (*struct*)
Becht, H.Y. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 3344 (*polymorphs*)
Deshpande, D.A. *et al*, *Thermochim. Acta*, 1983, **66**, 255 (*thermal dehydration, hydrate*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 606 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2896D; 2897A (*haz*)

IC-002734

CK_2S_3

Potassium trithiocarbonate

Trithiocarbonic acid, dipotassium salt, 8CI. Carbonotrithioic, acid, dipotassium salt, 9CI. Potassium thiocarbonate

[584-10-1]

K_2CS_3

M 186.4

Synth. by addition of H_2S to a satd. soln. of KOH, followed by pptn. with CS_2. Used in analysis, particularly for copper. Yellow-brown deliquescent orthorhombic cryst. Dec. on heating. V. sol. H_2O; spar. sol. EtOH; insol. Et_2O.

Silber, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **261**, 4126 (*synth*)
Philippot, E., *Rev. Chim. Minér.*, 1967, **4**, 643 (*ir*)
Philippot, E. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **268**, 1371 (*struct*)
Seidel, H., *Naturwissenschaften*, 1969, **56**, 212 (*uv*)

IC-002735

[CLa]

Lanthanum carbides

Lanthanum carbide ***(La_2C_3)*** [12076-36-7]
C_3La_2 M 313.8
Silvery yellow solid.

Lanthanum carbide ***(LaC_2)*** [12071-15-7]
Lanthanum dicarbide
C_2La M 162.9
Possesses CaC_2 struct. Converts lower alcohols to higher MW alcohols. Catalyst for hydrogenation of alkynes. Used in synth. of conductive ceramics. Brassy yellow solid. Mp 2438°. Dec. by H_2O affording principally C_2H_2, also C_2H_4, C_2H_6 and other hydrocarbons, $\alpha \rightarrow \beta$ transition 1060° (995°). LaC, La_2C also known.

Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 505 (*synth*)
Atoji, M., *J. Chem. Phys.*, 1961, **35**, 1950 (*struct*)
Palenik, G.J. *et al*, *Inorg. Chem.*, 1962, **1**, 345 (*reaction*)
Bowman, A.L. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 459 (*struct*)
Anderson, J.S. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 105 (*reactions*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **2**, 257 (*rev*)
Male, G., *Rev. Int. Hautes Temp. Refract.*, 1977, **14**, 179 (*synth*)
Gingerich, K.A. *et al*, *High Temp. Sci.*, 1981, **14**, 137 (*ms*)
Sakai, T. *et al*, *J. Chem. Phys.*, 1981, **75**, 3027 (*cond*)
Pelino, M. *et al*, *J. Chem. Phys.*, 1984, **80**, 4478 (*ms*)
U.S. Pat., 4 533 775, (1985); *CA*, **104**, 188658 (*use*)
Karen, P. *et al*, *Collect. Czech. Chem. Commun.*, 1986, **51**, 1411 (*synth, hydrol*)

IC-002736

CLiN

Lithium cyanide (LiCN), 8CI

[2408-36-8]

LiCN

M 32.9

Prepd. by reaction of HCN with Li dissolved in liq. NH_3 or by reaction of Li with AgCN (or $Hg(CN)_2$) in THF in presence of naphthalene. Alternatively obt. by reaction of BuLi in hexane with HCN in C_6H_6. Commercially available as solid or in soln. (0.5 *M*) in DMF. DMF solns. are effective reagents for halogen displacement. Catalyst for polym. of vinyl compds. White orthorhombic cryst. Reacts with acids with liberation of HCN. Forms a bis(THF) adduct. Mp 160°.

▷ Highly toxic.

Lely, J.A. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1942, **61**, 244 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No 20, 1960, 501 (*rev, bibl*)
Johns, I.B. *et al*, *J. Org. Chem.*, 1964, **29**, 1970 (*synth, uses*)
De Long, M.C. *et al*, *J. Crystal Growth*, 1986, **75**, 164 (*rev, synth*)

IC-002737

CLiNO

Lithium cyanate (LiOCN)

Cyanic acid, lithium salt, 8CI

[2363-79-3]

Li[OCN]

M 48.9

Ab initio calcs. of molecular LiOCN suggest it is linear. A similar conclusion is given by *ab initio* calcs. of molecular LiNCO but CNDO/2 calcs. of molecular LiNCO suggests bent LiNC and NCO angles. Manuf. by reaction of urea and Li_2CO_3 or by treatment of an alkylcarbamate with LiH in toluene. Prepd. by reaction in dry THF containing lithium naphthalide, of $LiAlH_4$ with AgOCN. Also prepd. by treatment of Li_2SO_4 with $Ba(OCN)_2$ obt. from NaOCN by reaction with $Ba(ClO_4)_2.6H_2O$. Colourless monoclinic cryst. V. sol. H_2O (68 g per 100 cm^3 at 25°). Mp 580-600°. ΔH_f° −478 kJ mol^{-1} (est).

U.S. Pat., 2 699 418, (1955); *CA*, **49**, 4930i (*synth, props*)
Valtr, Z. *et al*, *Z. Chem.*, 1966, **6**, 348 (*synth, ir*)
Rossmanith, K., *Monatsh. Chem.*, 1967, **98**, 501 (*synth*)
Nachbaur, E. *et al*, *Monatsh. Chem.*, 1973, **104**, 538 (*synth*)
Rode, B.M. *et al*, *Z. Naturforsch., A*, 1974, **29**, 650 (*theory*)
Poppinger, D. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3674 (*theory*)
Kaganyuk, D.S., *Zh. Neorg. Khim.*, 1978, **23**, 2003 (*thermochem data*)
U.S. Pat., 4 496 529, (1985); *CA*, **102**, 97735 (*synth*)

IC-002738

CLiNS

Lithium thiocyanate

Thiocyanic acid lithium salt, 8CI

[556-65-0]

LiSCN

M 65.0

Prepared by reaction of aq. $Ba(SCN)_2$ with aq. Li_2SO_4, or by slow neutralisation of Li_2CO_3 with thiocyanic acid. Component of absorbent-refrigerants used in solar refrigeration. Deliquescent white cryst. V. sol. H_2O.

▷ XL1540000.

Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 503 (*rev, bibl*)
Baddiel, C.B. *et al*, *Trans. Faraday Soc.*, 1964, **60**, 2009 (*raman*)
Chabanel, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1971, **272**, 253 (*ir*)
Gifford, M., *J. Chem. Soc., Perkin Trans. 2*, 1985, 157 (*cmr, N-15 nmr*)

IC-002739

CLi_2O_3

Lithium carbonate (Li_2CO_3)

Carbonic acid, dilithium salt, 8CI. Eskalith. Lithane. Lithobid. Lithonate. Lithotabs. NSC 16895. Camcolit. Priadel. Quilonum retard. Other synonyms

[554-13-2]

Li_2CO_3

M 73.8

Prep. by reaction of lithium formate and LiOH at 280°. Also formed by addition of aq. NH_3 and CO_2 to a conc. aq. soln. of LiCl. Commercially available. Used in treatment of manic depression. Dissolution in acids affords corresp. Li salts. Component of Li_2CO_3-Na_2CO_3-K_2CO_3 ternary eutectic used for fuel cell applications. Powder or white monoclinic cryst. Dec. on heating by CO_2 loss. Spar. sol. H_2O (1.5 g per 100 cm^3 at 0°; 0.7 g per 100 cm^3 at 100°); insol. EtOH, Me_2CO. Mp 720°. ΔH_f° −1216.0 kJ mol^{-1}; ΔG_f° −1132.1 kJ mol^{-1}; S° 90.2 J K^{-1} mol^{-1}.

▷ Toxic, corrosive. OJ5800000.

Zemann, J., *Acta Crystallogr.*, 1957, **10**, 664 (*cryst struct*)
U.K. Pat., 785 979, (1957); *CA*, **52**, 7633c (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 495 (*rev, bibl*)
Brooker, M.H. *et al*, *J. Chem. Phys.*, 1971, **54**, 4788 (*ir, raman*)
Coppen, A., *Biochem. Soc. Trans.*, 1973, **1**, 74 (*rev*)
Effenberger, H. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1979, **150**, 133 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 5057.
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 609 (*thermochem data*)
Stober, H.C., *Anal. Profiles Drug Subst.*, 1986, **15**, 367 (*rev, props, synth, pharmacol*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 12.
Hunter, R., *Br. J. Clin. Pharmacol.*, 1988, **25**, 375 (*pharmacol*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2152C.

IC-002740

CLi_4

Tetralithiomethane

Lithium carbide, 9CI

[38827-79-1]

CLi_4

M 39.7

Involatile solid, dec. >200°. Sl. sol. hexane in presence of di-*tert*-butylmercury.

Chung, C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1972, 1078 (*synth*)
Shimp, L.A. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 1343 (*synth*)
Collins, J.B. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 5419.
Shimp, L.A. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 5951 (*ms*)
Jemmis, E.D. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 4275 (*ms*)
Landro, F.J. *et al*, *J. Organomet. Chem.*, 1983, **249**, 1 (*synth*)
Chinn, J.W. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 3694 (*ms*)
Maercker, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 995 (*synth*)
Organomet. Synth., 1986, **3**, 378 (*synth*)

IC-002741

[CLu]

Lutetium carbides

Phases known include Lu_3C, LuC_2.

Lutetium carbide ***(LuC_2)*** [12175-89-2]
C_2Lu M 198.9
Possesses CaC_2 struct. Yellow solid. Dec. by H_2O. Undergoes $\alpha \rightarrow \beta$ transition at 1500° (1390°)(1450°).

Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 505 (*synth*)
Atoji, M., *J. Chem. Phys.*, 1961, **35**, 1950 (*struct*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)

IC-002742

$CMgO_3$

Magnesium carbonate, BAN, USAN

Carbonic acid, magnesium salt, 8CI

[546-93-0]

$MgCO_3$

M 84.3

Isotypic with $CaCO_3$ (calcite). Synth. from MgO + CO_2. Antacid. Used as an abrasive agent in toothpastes. White pigment. White powder; dec. on heating with CO_2 loss. Readily dissolves in aq. acids forming the corresp. salts. Prac. insol. H_2O (0.011 g per 100 cm^3); insol. Me_2CO, NH_3(l). Mp 350° dec. ΔH_f° −1112 kJ mol^{-1}; ΔG_f° −1028 kJ mol^{-1}; S° 65.9 J K^{-1} mol^{-1}.

▷ OM2470000.

Dihydrate: [5145-48-2]. *Barringtonite*
CH_4MgO_5 M 120.3
Triclinic cryst.

Trihydrate: [14457-83-1]. *Nesquehonite*
CH_6MgO_6 M 138.3
Monoclinic cryst. Spar. sol. H_2O (0.18 g per 100 cm^3 at 16°). Mp 165°.

Pentahydrate: [61042-72-6]. *Lansfordite*
CH_8MgO_8 M 172.3
Monoclinic cryst. Spar. sol. H_2O (0.38 g per 100 cm^3 at 20°). ΔH_f° −2584 kJ mol^{-1}.

Mineral-form [13717-00-5]
Magnesite
Member of calcite group of minerals. Occurrence widespread. Colourless to yellow to brown cryst.

[5145-46-0, 5145-47-1]

Fenoglio, M., *Atta Accad. Nazl. Lincei, Rend. Cl. Sci. Fis., Nat. Mat.*, 1936, **24**, 219 (*cryst struct, pentahydrate*)
Cohen, A. *et al*, *Helv. Chim. Acta*, 1939, **22**, 449 (*synth*)
Duval, R. *et al*, *Bull. Soc. Chim. Fr.*, 1943, 517 (*ir*)
Kinsolving, *et al*, *Am. Mineral.*, 1950, **35**, 127 (*cryst struct, trihydrate*)
Graf, D.L., *Am. Mineral.*, 1961, **46**, 1283 (*cryst struct*)
Vinogradova, L.M. *et al*, *Prib. Tekh. Eksp.*, 1971, 191; *CA*, **75**, 119239 (*uv*)
Belyaev, E.K. *et al*, *Zh. Fiz. Khim.*, 1978, **52**, 2709 (*ir, thermochem*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **14**, 618 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 698.
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 612 (*thermochem data*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2150.

IC-002743

[CMn]

Manganese carbides

Important in steel and as constituents of more complex metal alloys.

Manganese carbide ***($Mn_{23}C_6$), 11CI*** [12266-65-8]
C_6Mn_{23} M 1335.6
Cubic struct. consists of Mn-centred cuboctahedra of Mn and Mn cubes separated by C atoms. This is the only manganese carbide in which C occupies square antiprismatic voids. Isomorphous with $Cr_{23}C_6$. Synth. from Mn and graphite by sintering at 850° for 80h. Also formed from $Mn_2(CO)_{10}$ at 900° mixed with MnO and α-Mn. Antiferromagnetic between 90-400K, ferromagnetic at higher temps. $\mu_{eff} = 4.38\mu_B$ suggesting Mn^{+0} state. Reacts with oxygen, dec. in air in 20-40 h. Mp 1010°. ΔH_f° −245.5 kJ mol^{-1}; ΔS_f° 3.1 J K^{-1} mol^{-1}.

Manganese carbide ***($Mn_{15}C_4$), 10CI*** [12364-85-1]
C_4Mn_{15} M 872.1
The reported $Mn_{11}C_3$ was probably $Mn_{15}C_4.Mn_{15}C_4$ has also been considered to be Mn_7C_3. Synth. from Mn and graphite at 900-1000° in evacuated quartz ampoules for 12 h. Antiferromagnetic at 90-400K, ferromagnetic at higher temps., $\mu_{eff} = 4.01\mu_B$ suggesting the presence of Mn^{+0}. Hexagonal cryst. ΔG_f° −182 kJ mol^{-1} at 850°.

Manganese carbide ***(Mn_3C), 11CI*** [12121-90-3]
CMn_3 M 176.8
Struct. consist of sheets of corner and edge sharing trigonal CMn_6 prisms. Orthorhombic, isomorphous with Fe_3C. Synth. by heating the elements at *ca* 1300° for 3 h. Cheap Mn master alloy. Colour varies from yellow to silvery white. Hydrol. in H_2O to give H_2, CH_4, C_2H_6 and $Mn(OH)_2$. Mp *ca.* 1420°, Mp 1520°.
Antiferromagnetic, obeys Cure-Weiss law at 90-240K. At higher temps. becomes ferromagnetic. Upon hydrolysis a range of hydrocarbons is formed.

Manganese carbide ***(Mn_7C_3), 11CI*** [12071-17-9]
C_3Mn_7 M 298.7
Isomorphous with Pd_7B_3 and Fe_7C_3. Obt. by heating the elements at 700° in an evacuated quartz ampoule. Antiferromagnetic at 90-240K, ferromagnetic at higher temp. Monoclinic cryst. Readily reacts with O_2. A variety of hydrocarbons is formed upon hydrolysis. Mp *ca.* 1087°. ΔH_f° −69.96 kJ mol^{-1} for $2C_{sc} + 5Mn_{sc} \rightarrow Mn_7C_{3sc}$.

Manganese carbide ***(Mn_5C_2), 10CI*** [12076-37-8]
C_2Mn_5 M 420.5
Orthorhombic unit cell closely related to Ru_7B_3 and containing octahedra and tetrahedra of Mn atoms and C centred trigonal prisms. Most easily obt. manganese carbide from a melt since it is present in equilibrium with a Mn melt saturated with C. Can be prep. from the elements at 850° for 100h followed by heating to 1050° for 100h in evacuated quartz ampoules. Moisture and air-sensitive. Involatile up to 1025°. Mp 1150°. ΔG_f° −93.5 kJ mol^{-1}.

Manganese carbide ***(MnC), 10CI*** [12179-84-9]
CMn M 66.9
Does not exist as a stable crystalline compd. Amorphous MnC films have been obtained by sputtering pressed Mn—C mixtures at 77K.

Manganese carbide ***(MnC_2)*** [75718-05-7]
C_2Mn M 90.9
Hydrol. in H_2O giving H_2, CH_4 and C_2H_4.

Manganese carbide ***(Mn_2C_3)*** [75718-04-6]
C_3Mn_2 M 193.9
Orthorhombic, pseudohexagonal. Mp 1340°.

[12281-52-6, 12286-95-2, 12363-88-1, 12703-89-8, 37297-89-5, 39400-17-4, 60921-61-1, 112968-33-9, 114290-04-9]
Myers, W.R., *J. Am. Chem. Soc.*, 1945, **67**, 1962 (*synth, Mn_7C_3*)
Isobe, M., *CA*, 1953, **47**, 2585 (*phase diagram*)
Sénateur, J.P. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1962, **255**, 1815 (*synth, Mn_5C_2*)

Fasiska, E.J., *Acta Crystallogr.*, 1965, **19**, 463 (*cryst struct, Mn_3C*)
Bauchaud, J.P. *et al, Ann. Chim. (Paris)*, 1967, **2**, 353 (*synth, struct, $Mn_{15}C_4$*)
Frad, W.A., *Adv. Inorg. Chem. Radiochem.*, 1968, **11**, 153 (*rev*)
Nagakura, S. *et al, Trans. Iron Steel Inst. Jpn.*, 1968, **8**, 265 (*cryst struct, Mn_3C_2*)
Duggin, M.J., *Trans. Am. Inst. Min., Metall. Pet. Eng.*, 1969, **245**, 1347 (*struct, $Mn_{15}C_4$*)
Tanaka, H. *et al, CA*, 1972, **76**, 28487 (*thermodyn data*)
Lucco Barlero, M. *et al, CA*, 1972, **76**, 157350 (*synth $Mn_{23}C_6$*)
Ancy-Maret, M.F. *et al, CA*, 1973, **79**, 46358 (*thermodyn data*)
Benz, R., *Metall. Trans.*, 1973, **4**, 1449; 1974, **5**, 2217 (*thermochem data, phases struct, $Mn_{15}C_4$*)
Jeitschko, W., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1974, **5**, 219 (*cryst struct, $Mn_{23}C_6$*)
Hawarth, D.T. *et al, J. Inorg. Nucl. Chem.*, 1976, **40**, 1689 (*$Mn_{23}C_6$, cmr*)
Damasevich, L.T. *et al, CA*, 1977, **87**, 156088 (*hardness*)
Damasevich, L.T. *et al, Inorg. Materials (Engl. Transl.)*, 1977, **13**, 1733 (*magnetism*)
Arbuzov, M.P. *et al, CA*, 1978, **88**, 29763; 1980, **92**, 171885 (*electronic struct*)
Choudary, U.V. *et al, CA*, 1978, **88**, 118778 (*thermochem data*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 479, 500; **14**, 845.
Dawson, W.M. *et al, Metall. Trans. A*, 1980, **11**, 1849 (*thermochem data, $Mn_{23}C_6$*)
Hauser, J.J., *Phys. Rev. B*, 1980, **22**, 2554 (*synth, magnetism, struct, MnC*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 110 (*rev, bibl*)

$CMnN_3O_4$ IC-002744

Carbonyltrinitrosylmanganese, 8CI
[14951-98-5]

$Mn(NO)_3CO$

M 172.9
Synth. by photolysis of $Mn_2(CO)_{10}$ with NO. Green solid. Mp 27°.

Barraclough, C.G. *et al, J. Chem. Soc.*, 1960, 4842 (*synth*)
Inorg. Synth., 1976, **16**, 4 (*synth*)

$CMnN_4O_3^\ominus$ IC-002745

(Cyano-*C*)trinitrosylmanganate(1−)

$[(ON)_3MnCN]^\ominus$

M 170.9 (ion)
Na salt: [85962-31-8].
Synth. from $Mn(CO)(NO)_3$ and $NaN(SiMe_3)_2$ in C_6H_6. Grey-green solid. Ir ν_{CN} 2119s; ν_{NO} 1763m, 1662vs cm^{-1} (MeCN).
▷ Pyrophoric.

Moll, M. *et al, Z. Naturforsch., B*, 1983, **38**, 411 (*synth, ir*)

$CMnNa_3O_7P$ IC-002746

Sidorenkite
Sodium manganese(II) *carbonate phosphate* ($Na_3Mn(CO_3)(PO_4)$)
[70815-78-0]

$Na_3Mn(CO_3)(PO_4)$

M 278.8
Monoclinic with distorted MnO_6 octahedra linked together by PO_4 tetrahedra. Edge linking of CO_3 triangles with MnO_6 octahedra is unusual. Mn analogue of bradleyite ($Na_3MgCO_3PO_4$). Mineral, found in USSR. Transparent pale pink cryst.

Khomyakov, A.P. *et al, Am. Mineral.*, 1979, **64**, 1332.

Kurova, T.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1980, **251**, 605 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1983, **C9**, 237 (*rev, bibl*)

$CMnO_3$ IC-002747

Manganese(*II*) carbonate ($MnCO_3$)
[Carbonato(2−)-O]manganese, 11CI
[598-62-9]

$MnCO_3$

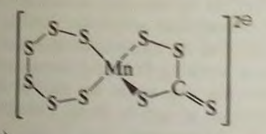
M 114.9
Calcite type struct., rhombohedral. Synth. by reaction of $Mn(OAc)_2.4H_2O$ solns. or $Mn(OH)_2$ with super critical CO_2 at 180° and 1200 atm. CO_2. Precipitation from aq. Mn^{+0} by $CO_3^{2\ominus}$ or $HCO_3^\ominus$ does not give stoichiometric pure products since CO_2 pressures are not high enough. Such products are of the type $Mn(CO_3)_x(OH)_y(H_2O)_z$. Pink to almost white powder. Commercial precipitated $MnCO_3$ is often light brown due to oxidation. Sol. saturated aq. K_2CO_3. Magnetically ordered below Néel temp. T_N 32.14K. $\mu_{eff} = 6.26\mu_B$. Dec. at 250-300°.

Mineral-form [14476-12-1]
Rhodochrosite
Found in e.g. Colorado USA, Romania, eastern Germany, South Africa. Pale pink to deep red or orangish cryst.

Amity, L. *et al, Phys. Lett. A*, 1968, **27**, 595 (*esr, nmr*)
Griffith, W.P., *J. Chem. Soc. A*, 1970, 286 (*ir, raman*)
Meijer, H.C. *et al, Physica (Amsterdam)*, 1970, **46**, 279 (*magnetism*)
McCain, W.S. *et al, Adv. X-Ray Anal.*, 1973, **16**, 390 (*cryst struct*)
Le Paillier-Malécat, A., *J. Phys. (Paris)*, 1973, **34**, 429 (*ur*)
Ehrhardt, H. *et al, Z. Anorg. Allg. Chem.*, 1980, **462**, 185; **465**, 83 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 174 (*rev, bibl*)

$CMnS_4^{2\ominus}$ IC-002748

[Carbono(dithioperoxo)dithioato(2−)-*S,S'*](hexathio) manganate(2−), 11CI
[83714-74-0]



M 387.6 (ion)
Bis-Ph_4P salt: Synth. from $[Ph_4P][Mn(S_3)(S_5)]$ and CS_2 in DMF. Orange-red air sensitive cryst. + DMF. Ir $\nu_{C=S}$ 905 cm^{-1}. Solns. turn blue-green upon exposure to air.

Coucouvanis, D. *et al, Inorg. Chem.*, 1985, **24**, 24 (*synth, ur*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 210 (*rev, bibl*)

CMn_5Si IC-002749

Manganese carbide silicide (Mn_5CSi), 11CI
[12274-91-8]

Mn_5CSi

M 314.7
$Mn_{21}Si_3C_4$ and $Mn_5Si_3C_x$ ($x \leqslant 0.22$) also exist. Synth. from elements in evacuated quartz ampoules at 700-1200°. Orthorhombic cryst. Transforms into a ferromagnetic order at 284K.

Spinat, P. *et al, Bull. Soc. Fr. Minéral. Cristallogr.*, 1970, **93**, 177; 1976, **99**, 13 (*synth, magnetism*)
Dubois, J.M. *et al, J. Solid State Chem.*, 1978, **24**, 189 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **C8**, 362 (*rev, bibl*)

CMn_6N IC-002750

Manganese nitride carbide, 10CI
[73963-94-7]
M 465.5
Typical formula given. Solid solns. of $Mn_4N_{1-x}C_x$ ($0 < x < 0.8$) are prepared from Mn_4N and unspecified manganese carbides at 1000°. Phases crystallise in perovskite structure of ε-Mn_4N.

Juza, R. *et al, Naturwissenschaften*, 1956, **43**, 225 (*synth, struct*)
Juza, R. *et al, Z. Elektrochem.*, 1957, **61**, 810 (*synth, struct*)
Takei, W.J. *et al, Phys. Rev.*, 1962, **125**, 1893 (*magnetism*)
Bauchaud, J.P. *et al, Bull. Soc. Chim. Fr.*, 1964, 1579 (*synth*)
Burglev, B.P., *CA*, 1967, **67**, 24159.
Bauchaud, J.P., *Ann. Chim. (Paris)*, 1968, **3**, 81 (*synth, struct, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 225 (*rev, bibl*)

[CMo] IC-002751

Molybdenum carbides
[12627-57-5]
Over 20 phases known.

Molybdenum carbide ***(Mo_6C)*** [12069-90-8]
CMo_6 M 587.6
Example of double carbide i.e. requires the integration of a second metal (e.g. Fe) to be stable. Obt. during treatment (tempering, quenching, annealing) of steels and alloys. Microconstituent and precipitant in steel and alloy matrices.

Molybdenum carbide ***($Mo_{2.2}C_x$)*** [12152-15-7]
$C_xMo_{2.2}$ M 2278.6
A double carbide. Formed during treatment of steels and alloys. Microconstituent and precipitant in steel and alloy matrices. Insol.

Molybdenum carbide ***(Mo_2C)*** [12069-89-5]
Molybdenum hemicarbide
CMo_2 M 203.8
Hcp array of Mo atoms, C atoms occupy half the octahedral holes between each pair of close packed layers. Synth. by many methods e.g. heating molybdenum powder and carbon black at about 1400-1500° under H_2. Used in cutting tools and other wear resistant surfaces, also in reactor and aerospace technology, owing to extreme hardness and high temp. stability. Oxidises on heating in air to MoO_3. Reacts with oxidising acids but not with dil. aq. alkali. Hard, electrical conductor exhibits superconductivity up to 2.9K. Insol. Mp 2687°.

Molybdenum carbide ***(MoC)*** [12011-97-1]
CMo M 107.9
Non-stoichiometric, possibly extending to Mo_3C_2 and lower; Mo_2C_2 also cited as alternative composition. Has a hexagonal lattice which resembles WC. Synth. by many methods e.g. heating Mo powder and carbon black at about 1400-1500° under hydrogen. Used in cutting tools and other wear-resistant surfaces, also in reactor and aerospace technology, owing to extreme hardness and high temp. stability. Oxidises on heating in

air to MoO_2 + CO_2. Reacts with oxidising acids but not dil. aq. alkali. Hard, electrical conductor, exhibits superconductivity, up to 7.9K. Insol. Mp 2692° prob. dec.

[11082-09-0, 12011-98-2, 12076-38-9, 12122-47-3, 12122-48-4, 12151-75-6, 12153-50-3, 12543-74-7, 87070-74-9, 110771-77-2, 112009-69-9, 116640-58-5, 116640-59-6, 117991-26-1, 117991-27-2, 124545-85-3, 124567-52-8, 124567-53-9, 126282-62-0, 130459-28-8]

Goldschmidt, H.J., *Interstitial Alloys*, Butterworths, London, 1967, 101 (*rev*)

Telegin, V.S. *et al*, *Kristallografiya*, 1967, **12**, 936 (*struct, Mo_2C*)

Cailler, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **270**, 1867 (*synth*)

Kolosova, E.L. *et al*, *Fiz. Met. Metalloved.*, 1970, **29**, 349 (*formn in steels*)

Storms, E.K., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. One*, 1971, **10**, 37 (*struct, phys props*)

Umanovshikov, Yu.I. *et al*, *Fiz. Met. Metalloved.*, 1978, **41**, 99 (*formn in steels*)

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 696; **19**, 58 (*uses*)

CNNa IC-002752

Sodium cyanide, 8CI

Cyanogran

[143-33-9]

NaCN

M 49.0

NaCl struct. Synth. by careful neutralisation of HCN with Na_2CO_3, $NaHCO_3$, or HCOONa. Manuf. by reaction of Na_2CO_3 and carbon with either N_2 or NH_3. Commercially available. Widely used in org. chem. for generation of C–C bonds. Colourless cubic cryst., deliquescent; undergoes cubic to hexagonal transition on cooling below 10.5°. V. sol. H_2O (48 g per 100 cm^3 at 10°; 82 g per 100 cm^3 at 35°); spar. sol. EtOH. Mp 562°. Bp 1496°. ΔH_f° −90.7 kJ mol^{-1}; ΔG_f° −80.4 kJ mol^{-1}; S° 118 JK^{-1} mol^{-1}.

▷ Highly toxic, irritant. VZ7525000.

Verweel, H.J. *et al*, *Z. Kristallogr.*, 1939, **100**, 201 (*cryst struct*)

Miller, F.A. *et al*, *Anal. Chem.*, 1952, **24**, 1253 (*ir*)

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 313; 1967, **4**, 137)

Kapperstein, C. *et al*, *Inorg. Chem.*, 1970, **8**, 2615 (*cmr*)

Tsuboya, A. *et al*, *Phys. Rev. Lett.*, 1980, **44**, 460 (*^{23}Na nmr*)

Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 616 (*thermochem data*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3137A (*haz*)

CNNaO IC-002753

Sodium cyanate

Cyanic acid, sodium salt, 8CI

[917-61-3]

NaOCN

M 65.0

Synth. by reaction of $Hg(OCN)_2$ and NaI in Me_2CO. Manuf. by oxidation of NaCN at 500-600° with O_2 or by treatment of a sodium salt (Na_2S, Na_2CO_3, NaCN, Na_2SO_3) with CO_2 or COS and NH_3. Commercially available. Cyclocondensation agent. Assessed for use in the therapy of sickle cell anaemia. Colourless hexagonal cryst. Sol. H_2O (10.7 g per 100 cm^3 at 16°); spar. sol. Et_2O, C_6H_6. ΔH_f° −400 kJ mol^{-1}. Dec. on heating to form NaCN, Na_2CO_3, N_2 and CO or CO_2 depending on temp.

▷ GS7000000.

West, C.D., *Z. Kristallogr.*, 1934, **88**, 97 (*cryst struct*)

Beck, W., *Chem. Ber.*, 1962, **95**, 341 (*ir*)

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1382 (*rev, bibl*)

Soderback, E., *Acta Chem. Scand.*, 1971, **25**, 3534 (*synth*)

Peterson, C.M. *et al*, *Semin. Hematol.*, 1974, **11**, 569 (*rev, therapy*)

U.S.S.R. Pat., 1 074 818, (1984); *C.A.*, **100**, 158962 (*manuf*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3136D (*haz*)

CNNaO IC-002754

Sodium fulminate

Fulminic acid, sodium salt, 8CI

[15736-98-8]

NaCNO

M 65.0

Synth. e.g. by shaking $Hg(CNO)_2$ with Na/Hg (3%) in absolute MeOH or EtOH under dry N_2. White salt. Readily (often explosively) dec. to form CO, N_2 and Na metal.

▷ Highly explosive: extreme caution must be exercised.

Beck, W., *Chem. Ber.*, 1962, **95**, 341 (*synth, ir*)

Iqbal, Z. *et al*, *Proc. R. Soc. London, A*, 1967, **302**, 35 (*synth, ir*)

Boddington, T. *et al*, *Trans. Faraday Soc.*, 1969, **65**, 500 (*thermal dec*)

Wentrup, C. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1970, **18**, 467 (*synth*)

Zeman, S. *et al*, *Thermochim. Acta*, 1984, **81**, 359 (*thermochem of dec*)

CNNaS IC-002755

Sodium thiocyanate

Thiocyanic acid, sodium salt, 8CI. Sodium sulfocyanate. Sodium rhodanide

[540-72-7]

NaSCN

M 81.0

Manuf. either by treatment of polysulfides (Na_2S_x) with NaCN or HCN or by heating NaSH with $(NH_2)_2CNCN$, or by reaction of sodium metal with thiourea. Commercially available. Used in thiocyanation reactions. Used in the electroplating industry and as a constituent of working fluids for energy storage and power generation. Aq. solns. are used in the final stages of the production of acrylic fibres. Colourless orthorhombic deliquescent cryst. V. sol. H_2O (139 g per 100 cm^3 at 21°; 225 g per 100 cm^3 at 100°); EtOH, Me_2CO. Mp 287°. ΔH_f° −174 kJ mol^{-1}.

▷ Toxic; irritant. XL2275000.

Rossini, F.D. *et al*, *Natl. Bur. Std. Circ. (U.S.)*, No. 500, 1952, 473 (*thermochem data*)

Rao, C.N.R. *et al*, *J. Sci. Ind. Res., Sect. B*, 1959, **18**, 169; *C.A.*, **53**, 19568i (*ir*)

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1387 (*rev, bibl*)

Van Rooyen, P.H. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 2933 (*struct*)

Kirillov, S.A., *Z. Phys. Chem. (Leipzig)*, 1978, **259**, 65 (*raman*)

Tabeta, R. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*^{23}Na nmr*)

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3156D (*haz*)

[CNNb] IC-002756

Niobium carbide nitride

[12687-87-5]

A number of compositions is known chiefly as constits. of alloys rather than pure phases. Composition tends to be variable and is often not specified.

Niobium carbide nitride (NbCN), 11CI [12274-94-1]

CNNb M 118.9

Manuf. by heating Nb nitride to 800-1000° in a CH_4 atm.

Jr. Pat., 1 508 370, (1968); *C.A.*, **70**, 59391b (*manuf*)

Sweeney, J., *Appl. Polym. Symp.*, 1977, **31**, 23 (*supercond, use*)

Christensen, A.N. *et al*, *J. Crystal Growth*, 1978, **44**, 353 (*single cryst*)

Liu, L.J. *et al*, *Appl. Phys. Lett.*, 1986, **49**, 416 (*synth, thin films*)

CNOTi IC-002757

Titanium carbide nitride oxide (TiCNO), 11CI

[71330-01-3]

TiCNO

M 89.8

Synth. only as coating on cutting tools by heating in H_2 + CH_4 + $TiCl_4$ at 710° or in hydrocarbon + N_2 + NH_3 + CO at 900-1100° or by chemical vapour deposition on silon. Forms a hard, wear resistant coating on cutting tools.

[6331-90-9]

Perry, A.J. *et al*, *Werkst. Ihre Verwdl.*, 1980, **2**, 335; *C.A.*, **94**, 126259)

Japn. Pat., 60 114 572, (1985); *C.A.*, **103**, 182648t (*use, synth*)

Japn. Pat., 60 238 482, (1985); *C.A.*, **104**, 154098s (*tool coating*)

CNOTl IC-002759

Thallium(I) cyanate

Thallium(I) isocyanate

TlNCO

M 246.4

Tetragonal, isomorphous with NaN_3. Obt. by mixing aq. solns. of NaNCO and TlOAc with addn. of EtOH. Predominantly ionic; diamagnetic. Sol. H_2O; sl. sol. EtOH.

▷ V. toxic.

Waddington, T.C., *J. Chem. Soc.*, 1959, 2499 (*struct, ir*)

CNRb IC-002760

Rubidium cyanide (RbCN), 8CI

[7073-56-4]

RbCN

M 111.4

Adopts NaCl-type struct. with disordered $CN^\ominus$ anions. Prepd. by addition of HCN mixed with C_6H_6 to RbOH dissolved in EtOH or similar non-aq. solv. Colourless cubic cryst. Hygroscopic. Moisture sensitive. Hydrol. to form either HCN and RbOH (< 50°) or NH_3 and HCOORb (> 80°). Transforms to a ferroelastically ordered monoclinic phase at −141°. Sol. H_2O; insol. EtOH, Et_2O. Mp 599°. ΔH_f° −117 kJ mol^{-1}.

▷ Highly toxic.

Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1965, **6**, 601 (*rev, uses*)

Sugisaki, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 1747 (*synth*)

Ladd, M.F.C., *Trans. Faraday Soc.*, 1969, **65**, 2712 (*thermochem data*)

Scavarda do Carmo, L.C. *et al*, *Phys. Rev. B*, 1981, **23**, 3186 (*e-*)

Ehrhardt, K.D. *et al*, *Acta Crystallogr., Sect. B*, 1983, **39**, 171 (*cryst struct, cubic form*)

Wasylishen, R.E. *et al*, *J. Chem. Phys.*, 1983, **78**, 1000 (*N-14 nmr*)

Eschner, S. *et al*, *Z. Phys. B:*, 1983, **52**, 37 (*N-14, 93-93, 85-87 nmr*)

Rowe, J.M. *et al*, *Phys. Rev. B*, 1984, **29**, 2168 (*cryst struct, ferroelastic form*)

Stroessner, K. *et al*, *J. Chem. Phys.*, 1985, **83**, 2435 (*high press polymorphs*)

Shimada, T. *et al*, *J. Chem. Phys.*, 1986, **85**, 3530 (*polymorphs*)

De Long, M.C. *et al*, *J. Crystal Growth*, 1988, **75**, 164 (*synth, props*)

CNSTl

Thallium(I) thiocyanate IC-002761

TlNCS

M 262.4

Orthorhombic isomorphous with KNCS. Synth. from thiocyanate ion + $Tl^\oplus$ (aq.). Colourless cryst. (H_2O). Sol. H_2O (0.0032 g per 100 cm^3); sl. sol. MeOH. ΔG, 38.5 kJ mol^{-1}. Dec. with dil. acid, reacts with excess $NCS^\ominus$ to give $Tl(NCS)_2^\ominus$ and $Tl(NCS)_3^{2\ominus}$.

▷ Toxic.

Golub, A.M. *et al*, *C.A.*, 1961, **55**, 23575 (*reactions*)

Patel, S.J., *J. Inorg. Nucl. Chem.*, 1970, **32**, 3708 (*synth ir, struct*)

CNSeTl IC-002762

Thallium(I) selenocyanate

Selenocyanic acid, thallium(1+) salt (1:1), 9CI, 8CI

[5162-67-4]

TlNCSe

M 309.3

Ionic. Synth. from TlOAc + KNCSe in EtOH. Yellow cryst.

▷ Toxic.

Mikitchenko, V.F. *et al*, *Ref. Zh. Khim.*, 1972, 7V97 (*sol, prod*)

[CNTi] IC-002763

Titanium carbide nitrides

[12627-33-7]

There is a substantial literature on these phases which have indeterminate compositions. Rel. little is known about stoichiometric compositions.

Titanium carbide nitride (TiCN), 11CI [12347-09-0]

CNTi M 73.8

Synth. by laser melting TiC and TiN or from TiO_2 or $TiCl_4$ in an RF or microwave plasma.

Titanium carbide nitride (Ti_2CN), 11CI [12654-86-3]

$CNTi_2$ M 121.7

Orthorhombic. Identified in Ti/C steels.

Titanium carbide nitride (Ti_4CN_3), 11CI [37242-48-1]

CN_3Ti_4 M 245.5
Synth. by heating the product of the reaction between TiBr in liq. NH_3 and Na acetylide. Formed in some steels.

Bold, T. *et al*, *Pr. Inst. Hutn.*, 1971, **23**, 159; *CA*, **77**, 42649p (Ti_4CN_3 *in steel*)
Fabritius, H. *et al*, *Arch. Eisenhuettenwes.*, 1974, **45**, 231 (*identification*, Ti_2CN)
Jeziorska, W., *Hutnick.*, 1976, **43**, 216; *CA*, **85**, 164351w (Ti_4CN_3 *in steel*)
Bolotov, A.V. *et al*, *Symp. Proc. - Int. Symp. Plasma Chem. 5th*, 1981, **2**, 850; *CA*, **97**, 167738m (*synth*, *TiCN*)
Japan. Pat., 61 17 471, (1986); *CA*, **105**, 47753z (*synth*, *TiCN*)
Maya, L., *Mater. Res. Soc. Symp. Proc.*, 1986, **73**, 401 (*synth*, Ti_4CN_3)

CNTl IC-002764

Thallium(*I*) cyanide

[13453-34-4]

TlCN

M 230.4
CsCl struct. Synth. from TlOPh with HCN in Et_2O suspension. Used in org. synth. for prep. of α-keto nitriles. Reacts with Me_3SiCl to give Me_3SiCN. Mod. sol. H_2O (16.8 g per 100 cm^3 at 28°).

▷ Toxic.

Matsuo, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1969, **42**, 1271 (*thermodynamics*)
Smith, D., *J. Phys. Chem.*, 1970, **74**, 2373 (*heat capacity*)
Taylor, E.C. *et al*, *J. Org. Chem.*, 1978, **43**, 2280 (*synth*)
L'vov, B.V. *et al*, *Prog. Anal. At. Spectrosc.*, 1980, **3**, 65 (*aa*)

[CNV] IC-002765

Vanadium carbide nitrides

[37232-24-9]

These phases are generally only found as components of steel alloys. A general preparation involves heating V_2O_5 in a mixture of CH_4, N_2 or NH_3, and H_2 at 900-1100°. Important as alloying components in tool steel and other high performance steels. Also used in ceramic composite cutting tools.

Vanadium carbide nitride* (*VCN*), *11CI [12069-91-9]
CNV M 76.9
Formed during rolling of austenitised steel or during annealing of quenched low-C steels.

Vanadium carbide nitride* (V_2CN), *11CI [62997-24-4]
CNV_2 M 127.9
Formed during annealing of quenched low-C steel.

Vanadium carbide nitride* (V_3CN), *11CI [101658-43-9]
CNV_3 M 178.8
Formed by heating steel with KCNO and K_2CO_3 at >500°.

Austrian Pat., 329 100, (1976); *CA*, **85**, 128451v (*synth*)
Schwaab, P., *Arch. Eisenhuettenwes.*, 1977, **48**, 163; *CA*, **86**, 192997a (*formn*, *VCN and* V_2CN)
Brown, E.L. *et al*, *Hot Deform. Austenite*, AIME, N.Y., 1977, 280; *CA*, **87**, 9354x (*form*, *VCN*)
Eur. Pat., 95 129, (1983); *CA*, **100**, 72990d (*ceram cutting tools*)
Cochaeva, T.I. *et al*, *Zashch. Pokrytiya Met.*, 1985, **19**, 72; *CA*, **104**, 172224b (*synth*, V_3CN)

[CNZr] IC-002766

Zirconium carbide nitrides

[12713-24-5]

Several compositions known. These phases may be synth. from $ZrCl_4 + NH_3 + CH_2Cl_2$, by heating $ZrO_2 + C + N_2$ at 1300-1500° or by heating ZrC + ZrN + Zr at 1800-2000°. Very hard; used alone or as alloys in abrasives and cutting tools; potential use in diamond polishing. Tested for use in solar energy conversion.

Zirconium carbide nitride* (*ZrCN*), *11CI [12601-90-0]
CNZr M 117.2
Synth. from ZrO_2, C and N_2 at 1600° for 2 hrs. An abrasive; also implicated in the weakening of low-alloy Zr steels in nuclear reactors.

Klimashin, G.M. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 843; *CA*, **77**, 53346p (*synth*)
Japan. Pat., 57 47 704, (1975); *CA*, **98**, 131290r (*diamond polishing*)
DeArdo, A.J. *et al*, *Mater./Metalwork Technol. Ser.*, 1975, **6**, 309.
Lyubimov, V.D. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1298 (*synth*)
Japan. Pat., 59 16 968, (1984); *CA*, **100**, 214501w (*manuf*)
Japan. Pat., 59 45 969, (1984); *CA*, **101**, 42510a (*synth*)
Japan. Pat., 61 19 777, (1986); *CA*, **104**, 172859u (*use*)
Bonnot, A.M. *et al*, *Sol. Energy Mater.*, 1986, **14**, 375 (*use*)

CN_2Ni IC-002767

Nickel(*II*) cyanamide

Ni(N=C=N)

M 98.7
Formed from $NiCl_2$ + NaCN with Fe catalyst. No recent reports.

Perret, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1937, **205**, 611.

CN_2Pb IC-002768

Lead(*II*) cyanamide

Cyanamide, lead(2+) salt (1:1), 9CI

[20837-86-9]

Pb(NCN)

M 247.2
Covalent struct. Synth. from CaNCN + $Pb(NO_3)_2$ or PbO. Also produced electrolytically using CaNCN/$NaClO_3$ and a Pb anode. Anticorrosive pigment in paints. Yellow cryst. Insol. H_2O.

[20890-10-2, 35112-70-0]

Bernard, M.A. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 2357 (*thermochem*)
Miyazaki, K., *Bull. Chem. Soc. Jpn.*, 1968, **41**, 1730 (*synth*)
Cooper, M.J., *Acta Crystallogr.*, 1964, **17**, 1449, 1452 (*synth*, *cryst struct*)

CN_2Tl_2 IC-002769

Thallium(*I*) cyanamide

$Tl_2[N=C=N]$

M 448.7
Synth. from aq. $NaCN_2$ and Tl_2SO_4. Red cryst. Mp 520°. Dec. at 275° giving $N_2 + C_2N_2$.

▷ Toxic.

Adams, K.M. *et al*, *Acta Crystallogr.*, 1964, **17**, 1449 (*struct*)
Siele, V.I. *et al*, *J. Chem. Soc.*, 1964, 6191 (*synth*, *dec*)

CN_4 IC-002770

Cyanogen azide

Cyanoazide

[764-05-6]

N≡C–N=N=N (C_s)

M 68.0
Interatomic distances; C≡N 116.4, C–N 138.9, CN=N 123.7, N=N 113.3 pm; angle CNN 121°. Synth. from NaN_3 + ClCN in CH_3CN. Oil.

▷ Detonates readily with great violence.

Marsh, F.D. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 4506 (*synth*)
Shurvell, H.F. *et al*, *J. Chem. Phys.*, 1970, **52**, 881 (*ir*, *microwave*)
Marsh, F.D., *J. Org. Chem.*, 1972, **37**, 2966 (*synth*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 323.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 2782.

CNa_2O_3 IC-002771

Sodium carbonate (Na_2CO_3)

Carbonic acid, disodium salt, 8CI. Soda ash

[497-19-8]

Na_2CO_3

M 105.9
Manuf. by the Solvay process in which aq. NaCl is converted by reaction with CO_2 and NH_3, into $NaHCO_3$ which is calcined to give Na_2CO_3. Alternatively produced by thermal dec. of the mineral trona, $Na_2CO_3.NaHCO_3.2H_2O$. Commercially available. Used in the paper pulp, soap and detergent industries; its principal application is as raw material for the production of glass. White monoclinic powder, hygroscopic. Dec. on heating by CO_2 loss. Undergoes monoclinic (β) to monoclinic (α) transition at 361° and monoclinic (β) to hexagonal (α) transition at 489°. V. sol. H_2O (7.1 g per 100 cm^3 at 0°; 46 g per 100 cm^3 at 100°); spar. sol. EtOH; insol. Me_2CO. Mp 850°. ΔH_f° −1130.8 kJ mol^{-1}; ΔG_f° −1048.0 kJ mol^{-1}; S° 138.8 JK^{-1} mol^{-1}.

▷ Irritant. VZ4050000.

Monohydrate: see *Sodium carbonate monohydrate*, *IC-002512*
Heptahydrate: see *Sodium carbonate* (Na_2CO_3) *heptahydrate*, *IC-002669*
Decahydrate: see *Sodium carbonate* (Na_2CO_3) *decahydrate*, *IC-002707*
Vratny, F. *et al*, *Appl. Spectrosc.*, 1960, **14**, 76 (*raman*)
Jardetzky, O. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 318 (*Na-23 nmr*)
Buijs, K. *et al*, *Spectrochim. Acta*, 1961, **17**, 927 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **18**, 458 (*rev*, *uses*)
Brouns, E. *et al*, *Acta Crystallogr.*, 1964, **17**, 614 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 267; 1966, **3**, 1317 (*rev*, *bibl*)
Clough, R.W., *Handb. Ind. Chem.*, 7th. Ed., 1974, 123 (*rev*, *uses*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 623 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3134D (*haz*)

[CNb] IC-002772

Niobium carbides

The more important phases are NbC and Nb_2C. No reaction with water; v. hard.

***Niobium carbide* (Nb_2C)** [12011-99-3]
CNb_2 M 197.8
Hcp niobium with ordered occupation of octahedral sites by C. Synth. by heating Nb + C to 2000° in high vacuum.

***Niobium carbide* (Nb_3C_2)** [12334-39-3]
C_2Nb_3 M 302.7
Hexagonal. Synth. by arc-melting using Nb and C electrodes.

***Niobium carbide* (Nb_4C_3)** [12076-39-0]
C_3Nb_4 M 407.6
The metals are close packed in a 12 layer sequence. Synth. by arc-melting Nb.

***Niobium carbide* (*NbC*)** [12069-94-2]
CNb M 104.9
There is a wide range of stoichiometry for this material. Has NaCl struct. but superstructures are also observed. Synth. by reducing Nb_2O_5 or NbO_2 with C, from $NbCl_5$ and CH_4 in an Ar–H_2 plasma or from ferro alloy and C-black at 1700-2000° in a vacuum furnace. Used in a wide variety of abrasives and cutting tools, in ceramics etc. and is formed in many Nb-containing alloys.

***Niobium carbide* (NbC_2)** [12188-72-6]
C_2Nb M 116.9
Struct. unknown but may be similar to CaC_2. Formed by pyrolysis of polycyclic aromatic compds. in the presence of Nb.

Becker, K. *et al*, *Z. Phys.*, 1925, **31**, 268 (*cryst struct*, *NbC*)
Yvon, K. *et al*, *Monatsh. Chem.*, 1967, **98**, 34 (*synth*, *cryst struct*, Nb_2C)
Yvon, K. *et al*, *Acta Crystallogr., Sect. B*, 1970, **26**, 149 (*synth*, *cryst struct*, Nb_4C_3)
Crane, R.L. *et al*, *Metall. Trans.*, 1971, **2**, 3487 (*synth*, *struct*, Nb_3C_2)
Binder, F. *et al*, *Radex Rundsch.*, 1981, 690; *CA*, **96**, 204273h (*manuf*, *NbC*)
U.K. Pat., 2 065 652, (1981); *CA*, **96**, 35217k (*synth*, NbC_2)
Blagoveshchenskii, Yu.V. *et al*, *Fiz. Khim. Obrab. Mater.*, 1982, 32; *CA*, **98**, 94446g (*synth*, *NbC*)
Ouensangi, A., *J. Less-Common Met.*, 1986, **119**, 189 (*synth*, *NbC*)

[CNd] IC-002773

Neodymium carbides

Known phases include Nd_2C_3, NdC_2.

***Neodymium carbide* (NdC_2)** [12071-21-5]
C_2Nd M 168.2
Has CaC_2 struct. Brassy yellow solid. Mp 2340° dec. Dec. by H_2O, affording mainly C_2H_2 but also C_2H_4, C_2H_6 and other hydrocarbons. Undergoes α→β transition at 1150°. $\mu_{eff} = 3.53\mu_B$ (θ +40°). Antiferromagnetic (T_N 29K).

Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth*, *struct*)
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 503, 505 (*synth*, *magnetism*)
Atoji, M., *J. Chem. Phys.*, 1967, **46**, 1891 (*magnetism*)
Anderson, J.S. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 105.
McColm, I.J. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1931 (*synth*, *props*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Male, G., *CA*, 1976, **85**, 153174; *CA*, 1978, **88**, 44271 (*synth*)
Wegener, W. *et al*, *Cryst. Electr. Field Eff. f-electron Magn., [Proc. Int. Conf., 4th]*, 1982, 185; *CA*, 1983, **98**, 60124 (*magnetism*)
Jones, D.W. *et al*, *J. Solid State Chem.*, 1986, **62**, 172 (*cryst struct*, NdC_2)

[CNi]

IC-002774

Nickel carbides

[12710-36-0]

Widely used as a catalyst, e.g. in the conversion of exhaust gas. Occurs in various formulations in solid solns. and phase systems with other metal carbides. The most common formulation is Ni_3C.

Nickel carbide (Ni_3C) [12012-02-1]

CNi_3 M 188.0

Fe_3C struct. Has cubic and hexagonal phases. Dark grey powder.

[12152-16-8, 12167-08-7, 12601-91-1, 37297-90-8, 52931-58-5, 94559-70-0, 107069-48-7]

Kostjan, B.I. et al, Fiz. Tverd. Tela (Leningrad), 1975, 73 (forms)
Baird, T., Carbon, 1977, 15, 379 (synth)
Elshova, T.P. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1981, 4, 201 (Ni/C phase syst)
L'vyanol, V.N. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1981, 5, 161 (synth, pe)
Baranova, R.V. et al, Kristallografiya, 1982, 27, 923 (struct)

$CNiO_3$

IC-002775

Nickel(III) carbonate ($NiCO_3$)

[3333-67-3]

$NiCO_3$

M 118.6

Structs. unknown. Synth. from Nickel(II) chloride ($NiCl_2$), IC-018717 + $CaCO_3$ at 150° in sealed tube. Light green solid.

▷ QR6200000.

Hexahydrate: Hellyerite

Synth. from Hexaaquanickel(II)(2+), IC-019897 + $NaHCO_3$, or obt. as mineral from old Lord Brassey nickel mine, Tasmania. Pale green or blue fine vitreous cryst.

Basic carbonate: [29863-10-3]. Nickel carbonate hydroxide. Basic nickel carbonate

Synth. from Hexaaquanickel(II)(2+), IC-019897 + Na_2CO_3. Commercially available; used to synth. other Ni compds. by reaction with acids; used in ceramic pigments. Approx. formula $Ni_4(OH)_6(CO_3)_2.4H_2O$. Also formulated as $2NiCO_3.3Ni(OH)_2.4H_2O$. Other undefined basic nickel carbonates known.

Sidgwick, N.V., The Chemical Elements and their Compds., 1950, 1435.
Remy, H., Treatise on Inorg. Chem., Elsevier, 1956, 2, 316.
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1966, B3, 840, 852 (rev, bib)
Brauer, G., Handbuch Prdp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 3, 1897 (synth)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 15, 804 (uses)

[CNp]

IC-002776

Neptunium carbides

Three main phases: Np_2C_3, NpC, NpC_2.

Neptunium carbide (Np_2C_3) [12347-28-3]

C_3Np_2 M 510.1

Isostruct. with Pu_2C_3, Am_2C_3. Ferromagnetic <109K.

Neptunium carbide (NpC) [12240-17-4]

CNp M 249.0

NaCl struct. Antiferromagnetic between 220-310K. Ferromagnetic below 220K (190K). $\mu_{eff} = 2.1\mu_B$ (6-150K).

Neptunium carbide (NpC_2)

C_2Np M 261.0

Tetragonal CaC_2 struct.

Sheft, I. et al, J. Am. Chem. Soc., 1953, 75, 1236 (synth, struct)
Lorenzelli, R., Compt. Rend. Hebd. Seances Acad. Sci. Sect. C, 1968, 266, 900 (synth)
DeNorion, C.H. et al, J. Phys. Chem. Solids, 1968, 29, 1901 (magnetism)
Lander, G.H. et al, J. Phys. Chem. Solids, 1969, 30, 733 (synth, ed, NpC)
Mitchell, A.W. et al, J. Nucl. Mater., 1970, 36, 110 (cryst struct)
Dunlop, B.D. et al, J. Appl. Phys., 1971, 42, 1719 (magnetism)
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, C, 189 (rev)
Brauer, G., Handbuch Prdp. Anorg. Chem., 3rd Ed, Ferdinand Enke Verlag, 1975-1981, 2, 1275, 1276 (synth, NpC, Np_2C_3)
Mallett, C.P., J. Phys. Chem., 1982, 15, 6361 (ed, struct)
Holleck, H., Handbook on the Physics and Chemistry of the Actinides, (Freeman, A.J., et al, Eds.), 1986, 4, 209 (rev)

CO

IC-002777

Carbon monoxide

[630-08-0]

CO

M 28.0

Interatomic distance C—O 112.8 pm. Manuf. by partial oxidn. of hydrocarbon gases from natural gas, or gasification of coke and coal. Synth. from HCO_2H + H_2SO_4. Prod. in traces by algae and higher plants. Reducing agent, used in Fischer-Tropsch processes for petroleum-type products, manuf. of metal carbonyls. Carbonylates organoboranes. Commercially available. Odourless, tasteless, colourless gas. V. spar. sol. H_2O; sol. AcOH, MeOH, EtOH. Mp −213°. Bp −190°. Crit. point −114.1° (−138.7°)/35.9 atm. Readily absorbed by conc. solns. of Cu_2Cl_2 in aq. NH_3 or HCl. Exhaust gas, air pollutant.

▷ Highly toxic by inhalation. TLV 55. Extremely flammable, forms highly explosive mixtures with air. FG3500000.

Mellor, J.W., Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1922, 5, 921, 925, 945 (bib)
Inorg. Synth., 1946, 2, 81 (synth)
Weinhouse, S., J. Am. Chem. Soc., 1948, 70, 442 (synth)
Wilks, S.S., Science (Washington, D.C.), 1959, 129, 964 (occur)
Siegel, S.M. et al, Science (Washington, D.C.), 1962, 137, 683 (occur)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, 2, 80,204; 3, 41; 5, 96; 7, 53; 8, 76; 9, 95; 11, 111 (uses)
Brauer, G., Handbuch Prdp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 621 (synth)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 4, 772 (rev)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, 8, 76.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 230.
Sax, N.I. et al, Dangerous Properties of Industrial Materials, 7th Ed., Van Nostrand-Reinhold, 1989, 713 (haz)

COS

IC-002778

Carbonyl sulfide

Carbon oxide sulfide, 9CI. Carbon oxysulfide. Thiocarbonic anhydride

[463-58-1]

O═C═S ($C_{\infty v}$)

M 60.0

Interatomic distances: C—O 115.7 C—S 156.1 pm. Isol. from roots of *Cochlearia armoracia*. Synth. from CO + S. Commercially available in cylinders. Used in C-

carboxylation of enolates. Colourless gas, hydrol. by H_2O. V. sl. sol. H_2O; sol. EtOH, toluene. d^{-50} 1.19. Mp −138.2°. Bp −50.2° (−47.5°). T_c 105°, P_c 58.68 atm. Dec at 900° to CO + S.

▷ Highly toxic by inhalation, irritant. Explosive in air, flammable. FG6400000.

Mellor, J.W., Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1922, 5, 971 (bib)
Francis, F.G. et al, J. Chem. Soc., 1932, 660 (props)
Schildknecht, H., Z. Naturforsch., B, 1962, 17, 800 (tool)
Morino, Y. et al, Bull. Chem. Soc. Jpn., 1967, 40, 1095 (struct)
Finn, E. et al, J. Mol. Spectrosc., 1975, 56, 39 (struct)
Brauer, G., Handbuch Prdp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 625 (synth)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 22, 107 (rev)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1984, 11, 112 (use)
Sax, N.I. et al, Dangerous Properties of Industrial Materials, 7th Ed., Van Nostrand-Reinhold, 1989, 718 (haz)

COSe

IC-002779

Carbonyl selenide

Carbon oxide selenide

[1603-84-5]

O═C═Se ($C_{\infty v}$)

M 106.9

Interatomic distances: O—C 115.7, C—Se 170.9 pm. Synth. by reaction of CO + Se at 400° or by reaction of Al_2Se_3 + CO at 219°. Colourless foul smelling gas, hydrol. by H_2O.

Gmelin, O. et al, Z. Naturforsch., B, 1948, 3, 1.
Morino, Y. et al, Bull. Chem. Soc. Jpn., 1967, 40, 1101 (struct)
Finn, E. et al, J. Mol. Spectrosc., 1975, 56, 39, 52 (struct)
Brauer, G., Handbuch Prdp. Anorg. Chem., 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 626 (synth, bib)

COTe

IC-002780

Carbonyl telluride

[2202-31-5]

Te═C═O

M 155.6

Synth. from Te + CO (low yield). Gas.

Robinson, P.L. et al, Nature (London), 1944, 153, 24 (synth)
Williams, E.J. et al, J. Mol. Struct., 1968, 2, 57 (theory)

[COTi]

IC-002781

Titanium carbide oxides

[12688-08-3]

Much work has been reported on Ti—C—O phases of indeterminate composition. Rather little is known of stoichiometric phases. All phases find their major use as coatings for cutting tools.

Titanium carbide oxide ($TiCO$), 11CI [12539-68-3]

COTi M 75.8

Synth. from TiC and TiO at 1500°. Component in anodes for Al electrowinning.

Titanium carbide oxide (Ti_2CO), 11CI [11086-75-2]

$COTi_2$ M 123.7

Ordered NaCl struct. over entire composition range. Synth. by heating TiC and TiO or by reaction of a mixture of $TiCl_4$, H_2, CO_2, CO and CH_4. Used to improve strength of sintered ceramic bodies.

Kamyshov, V.M. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1972, 8, 1185; CA, 77, 106261r (cryst struct, phase stability, Ti_2CO)
Viana, J. et al, Rev. Chim. Minér., 1972, 9, 557 (synth, phase stab, TiCO)
Carson, W.W. et al, J. Eng. Ind., 1976, 98, 279; CA, 85, 128738 (synth, Ti_2CO)
Kikuchi, N. et al, Proc. Electrochem. Soc., 1977, 77-75, 403 (synth, use, Ti_2CO)
U.S. Pat., 4 187 155, (1980); CA, 92, 155122q (use, TiCO)
Japan. Pat., 60 159 171, (1985); CA, 104, 23175t (use, TiCO)
Japan. Pat., 60 180 958, (1985); CA, 104, 173162r (use, Ti_2CO)

[COZr]

IC-002782

Zirconium carbide oxide, 11CI

[12651-47-7]

$ZrO_{0.15}C_{0.85}$

Non-stoichiometric with respect to C and O. Several phases known, with the NaCl struct. having vacancies on one or both sub-lattices in the composition range ZrC_xO_y where $x + y = 0.4$-0.5 and $y \leq 0.15$. These phases may be synthesised (a) on a Zr surface (b) by heating ZrO_2 + C black at 1250-1500°, (c) by heating ZrC + ZrO_2 + Zr *in vacuo* at 1800-2000°. Potential absorbers for solar energy systems.

Alyamovskii, S.I. et al, Russ. J. Inorg. Chem. (Engl. Transl.), 1971, 16, 3 (cryst struct)
Klimashin, G.M. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1972, 8, 843; CA, 77, 53340p (synth)
Zainulin, Yu.G. et al, Russ. J. Inorg. Chem. (Engl. Transl.), 1973, 18, 1052 (cryst struct)
Lyubimov, V.D. et al, Izv. Akad. Nauk SSSR Neorg. Mat., 1976, 12, 2159; CA, 86, 83061v (synth)
Blickensderfer, R. et al, Rep. Invest.: U.S., Bur. Mines, 1978, 8357; CA, 88, 93862k (use)
Uglov, A.A. et al, Fiz. Khim. Obrab. Mater., 1985, 140; CA, 103, 204741x (synth on Zr surface)

CO_2

IC-002783

Carbon dioxide

Carbon oxide (CO_2). Carbonic anhydride

[124-38-9]

O═C═O ($D_{\infty h}$)

M 44.0

Final oxidation product of carbon. Forms part of the carbon cycle in nature Interatomic distance C—O 115.98 pm. Used in carbonation of beverages, manuf. of carbonates, fire prevention and extinction, propellant (aerosols), antiseptic in bacteriology and in frozen food ind. Respiratory stimulant. Commercially available in cylinders and as solid at −78°(Dry ice). Important in 'greenhouse effect' and photosynthesis. Colourless odourless gas. Reduced to CO by C or H_2. Dissociates above 2000° to CO + O_2. Spar. sol. H_2O, forming H_2CO_3. d 1.52(0) (air = 1). Mp −57° under 5 atm. Bp −78.2°, Bp −78.5°, Sublt. −78.46°. Liquifies at 20° under 50 atm. pressure. Aq. soln. is acid to litmus. Crit. point 31.3°/72.9atm. Triple pt. −56.6° at 5.11 atm.

▷ Solid causes skin burns. FF6400000.

Jaeglé, A. et al, J. de Chimie Physique, 1970, 67, 467 (struct)
Gay, I.D. et al, J. Phys. Chem., 1974, 78, 58 (rev)
Perizzo, J.J., CA, 1975, 82, 177523b (ir)
Brauer, G., Handbuch Prdp. Anorg. Chem., 3rd Ed., Academic Press, N.Y., 1975-1981, 2, 622 (synth)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, 4, 725 (rev)
Clark, W.C., Ed., Carbon Dioxide Review 1982, Oxford Univ. Press, N.Y., 1982 (rev)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 1202.

Behr, A., *Angew. Chem., Int. Ed. Engl.*, 1988, **27**, 661 (*rev, use*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 229.

IC-002784

CO_3Pb

Lead(*II*) carbonate ($PbCO_3$)

Carbonic acid, lead(2+) salt (1:1), 9CI

[598-63-0]

$PbCO_3$

M 267.2

Prepd. by passing CO_2 into a dilute soln. of $Pb(OAc)_2$. Cryst. Spar. sol. H_2O; insol. EtOH. Mp 315° dec.

▷ Toxic. OF9275000.

Mineral-form [14476-15-4]

Cerussite

Occurs widely as secondary mineral. Colourless, white, grey, smoky; sometimes blue, green, dark grey or black due to inclusions.

Lemke, A. *et al*, *Z. Anorg. Allg. Chem.*, 1934, **220**, 312 (*synth*)
Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1951, **2**, 200 (*mineralogy*)
Miller, F.A. *et al*, *Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1970, 286 (*raman*)
Andreeva, V.A. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 2089; *CA*, **73**, 115181c (*synth*)
Sahl, K., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1974, **139**, 215 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1981, **14**, 171 (*rev*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2100.

IC-002785

CO_3Rb_2

Rubidium carbonate (Rb_2CO_3)

Carbonic acid, dirubidium salt, 8CI

[584-09-8]

Rb_2CO_3

M 230.9

Prepd. from aq. RbOH + CO_2 at 1000-2200 atm. and 200-400°. Alternatively an aq. soln. of RbOH, obtained by reaction of Rb_2SO_4 with $Ba(OH)_2$, is treated with $(NH_4)_2CO_3$. Commercially available. Catalyst for gasification of graphite. Dissolution in acids affords the corresp. Rb salts. Colourless monoclinic cryst.; deliquescent. Dec. on heating with CO_2 loss. V. sol. H_2O (450 g per 100 cm^3 at 20°). Mp 837° (> 1 atm). ΔH_f° −1136 kJ mol^{-1}; ΔG_f° −1051 kJ mol^{-1}; S° 181 J K^{-1} mol^{-1}.

▷ Irritant; corrosive.

Gmelin Handbook Inorg. Chem., Syst. No. 24, 1955, 222 (*rev, bibl*)
Brooker, M.H. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 2211 (*ir, raman*)
Ehrhardt, H. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **462**, 185 (*synth, cryst struct*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3056C.

IC-002786

CO_3Sr

Strontium carbonate ($SrCO_3$)

Carbonic acid, strontium salt, 8CI

[1633-05-2]

$SrCO_3$

M 147.6

Manuf. from celestite by treatment with either aq. Na_2CO_3 or aq. $(NH_4)_2CO_3$. Commercially available. Used in the synthesis of ternary oxides by reaction with transition metal oxides. Colourless orthorhombic cryst. Dec. on heating with CO_2 loss. Orthorhombic to hexagonal phase transition at 925°. Pract. insol. H_2O (0.0011 g per 100 cm^3 at 18°; 0.065 g per 100 cm^3 at 100°). Mp 1497° (65 atm.). ΔH_f° −1220.1 kJ mol^{-1}; ΔG_f° −1140.4 kJ mol^{-1}.

Mineral-form [14941-40-3]

Strontianite

Member of the aragonite ($CaCO_3$) group of minerals. Occurs as low temp. mineral as veins in limestones and marls. White or yellowish cryst.

Swanson, H.E. *et al*, *Natl. Bur. Std. Circ.* (*U.S.*), 1954, **3**, 56 (*cryst struct*)
Angelov, I.I. *et al*, *CA*, 1959, **53**, 8903i (*purif*)
Krishnamurti, D., *Proc. - Indian Acad. Sci., Sect. A*, 1960, **51**, 285 (*raman*)
Baker, E.H., *J. Chem. Soc.*, 1962, 2525 (*polymorph*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **19**, 50 (*uses*)
Witzmann, H. *et al*, *CA*, 1964, **61**, 1485a (*synth*)
Ross, S.D. *et al*, *Spectrochim. Acta*, 1964, **20**, 781 (*ir*)
Criado, J.M. *et al*, *Thermochim. Acta*, 1980, **38**, 117 (*thermal dec*)

IC-002787

$[CO_3Tc]$

Carbonate technetium complex

Technetium carbonate complex

$CO_3^{2\ominus}$ + Tc

Several complexes $[Tc(OH)_n(CO_3)_m]^{z\ominus}$ appear to exist, involving Tc^{III} and Tc^{IV}. A well-defined thiocarbonate species $[TcN(S_2CO)_2]^{2\ominus}$ has been reported.

Paquette, J. *et al*, *Can. J. Chem.*, 1985, **63**, 2369 (*spectroelectrochem*)
Rossi, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1990, 2923 (*analogue*)

IC-002788

CO_3Tl_2

Thallium(*I*) carbonate (Tl_2CO_3)

Thallous carbonate

[6533-73-9]

Tl_2CO_3

M 468.7

Monoclinic at r.t. (γ-form), transforms to α-form at 200° and to β-form at 263°. Obt. by action of CO_2 on aq. TlOH. Colourless needles, stable in air to 175°, loses CO_2 on further heating, dissolves acidic oxides. Sol. H_2O; insol EtOH. Mp 272°.

▷ V. toxic. XG4000000.

Mitchell, A., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1966, **123**, 399 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 884 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1984, **11**, 515 (*use*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3238 (*tox*)

IC-002789

CO_3Zn

Zinc carbonate ($ZnCO_3$)

[3486-35-9]

$ZnCO_3$

M 125.3

Calcite struct. Mineral formed on zinc during atmospheric corrosion. Used in deodorants; blowing agent; polym. catalyst; fireproofing agent; flame retardant; nutrient and feed supplement; filler and binder; pigment. Rhombohedral colourless cryst. Pract. insol. H_2O (5.7 × 10^{-5} g per 100 cm^3). Dec. at 140°. Forms a basic salt on boiling in H_2O.

▷ FG3375000.

Mineral-form

Smithsonite

Secondary mineral, often found as grape-like clusters, or crystalline crusts. Widespread occurrence. Trigonal cryst., rarely colourless, ranges from bright apple green to deep pink purple.

Hüttig, G.F. *et al*, *Monatsh. Chem.*, 1939, **72**, 31.
Gmelins Handbook Inorg. Chem., Syst. No. 32, 1956, 973.
Graf, D.L., *Am. Mineral.*, 1961, **46**, 1283 (*powder struct*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **22**, 604.
Cibor, E. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1964, **38**, 1715 (*synth, powder struct*)
Donoghue, M. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 1065 (*ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1035 (*synth*)

IC-002790

CO_4Zr

[Carbonato(2−)-*O,O'*]oxozirconium(*IV*), 11CI

Zirconium(IV) *carbonate oxide*

[15667-84-2]

$ZrO(CO_3)$

M 167.2

May be synth. from aq. solns. of $ZrOSO_4$ and either Na_2CO_3 or $(NH_4)_2CO_3$. Used in the preparation of ultrafine ZrO_2, in improving H_2O and abrasion resistance in wool and in waterproofing silicate building materials. Commercially available. White solid.

[34842-61-0, 37356-18-6]

Japan. Pat., 71 27 552, (1971); *CA*, **76**, 35172d (*catalyst*)
Ger. Pat., 2 510 743, (1975); *CA*, **84**, 61961v (*synth*)
Japan. Pat., 75 24 974, (1975); *CA*, **84**, 94696r (*proofing silicates*)
Ehrhardt, H. *et al*, *Z. Anorg. Allg. Chem.*, 1980, 462, 185 (*synth*)
Japan. Pat., 59 46 129, (1984); *CA*, **101**, 97634z (*medical use*)
Zhang, Y.-C. *et al*, *J. Less-Common Met.*, 1986, **116**, 301 (*use*)

IC-002791

CO_4U

Uranyl(*VI*) carbonate

[*Carbonato*(2−)-O]*dioxouranium*(VI)

[12274-95-2]

$UO_2(CO_3)$

M 330.0

8-Coord. (2 + 6), U—O 167 pm. Green-yellow or yellow to brown orthorhombic cryst. Sl. sol. H_2O. Dec. to CO_2 + UO_3 at 500°. Reduced to UO_2 by HCHO. Ir ν_{OUO} 965 cm^{-1}.

Mineral-form [63890-22-2]

Rutherfordine

Sometimes occurs as hemihydrate. Occurs at sites in Africa, USA. and Australia. White, pale yellow to amber orthorhombic cryst.

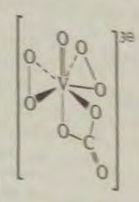
[12202-79-8, 13021-32-4]

Cromer, D.T. *et al*, *Acta Crystallogr.*, 1955, **8**, 847 (*cryst struct*)
Christ, G.L. *et al*, *Science* (*Washington, D.C.*), 1955, **121**, 472 (*cryst struct*)
Blake, C.A. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 5978 (*synth, props*)
Chernyaev, I.I. *et al*, *Zh. Neorg. Khim.*, 1956, **1**, 2726 (*synth*)
Cejka, J., *Chem. Listy*, 1960, **54**, 124 (*rev*)
Hoekstra, H.R., *Inorg. Chem.*, 1963, **2**, 492 (*synth, ir*)
Warren, I.H. *et al*, *J. Appl. Chem.*, 1963, **13**, 101 (*synth*)
Veal, B.W. *et al*, *Phys. Rev. B*, 1975, **12**, 5651 (*pr*)
Čejka, J. *et al*, *J. Therm. Anal.*, 1977, **12**, 117 (*dta*)
U.S.S.R. Pat., 560 832, (1977); *CA*, **87**, 103931 (*manuf*)
U.S. Pat., 4567, 025, (1986); *CA*, **104**, 118293 (*use*)

$CO_8V^{3\ominus}$

[Carbonato(2−)-*O,O'*]oxodiperoxyvanadate(*V*)(3−), 11CI

IC-002792



M 190.9 (ion)

Pentagonal bipyramidal. V is displaced 36 pm towards the axial $O^{2\ominus}$.

Tri-Na salt: [103065-13-0].

Synth. analogous to K salt. Yellow solid.

Tri-K salt: [74994-35-7].

Synth. e.g. by dissolving K_2CO_3 and V_2O_5 in 30% H_2O_2. Yellow solid.

[92538-86-8]

Schwendt, P. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **466**, 232 (*synth from KVO_3*)
Stomberg, R., *Acta Chem. Scand., Ser. A*, 1985, **39**, 725 (*cryst struct K salt*)
Basumatary, J.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 709 (*synth from V_2O_5, ir, raman, K, Na salt trihydrates*)

IC-002793

CPV_2

Vanadium carbide phosphide (V_2CP), 9CI

[12340-48-6]

V_2PC

M 144.8

Synth by heating the elements to 1000° in a sealed silica tube.

Boller, H. *et al*, *Monatsh. Chem.*, 1973, **104**, 48; 1968, **99**, 672 (*synth, cryst struct*)

IC-002794

[CPa]

Protactinium carbides

[61008-51-3]

Protactinium carbide (***PaC***) [12539-76-3]

CPa M 243.0

Has NaCl struct. Reaction with I_2 has been used in mod. van-Arkel synth. of Pa. Reacts with $SOCl_2$, Br_2, HgI_2 on heating to afford Pa halides. Air-stable solid. Magnetic measurements show temp. independent paramag. Compd. possibly Pa(*V*) i.e. $Pa^{5\oplus}(C^{4\ominus})e^{\ominus}$.

Protactinium carbide (***PaC_2***)

C_2Pa M 255.0

Tetragonal cryst.

Lorentz, R. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 2381.
Lindner, R., *Nucl. Sci. Abstr.*, 1969, **23**, 26984; 1971, **25**, 45113; *CA*, **71**, 97891; *CA*, **76**, 9485 (*struct*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **5**, 357 (*rev*)
Brown, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1336 (*use*)
Heny, Y. *et al*, *Proc. - Int. Conf. Electron. Struct. Actinides, 2nd, 1976*, 1976, 343; *CA*, **87**, 32938, 77600 (*magnetism*)
*Gmelin Handbook Inorg. Chem., Syst. No.*51, *Supplement Vol.2*, 1977, 80 (*rev, bibl*)
Mallet, C.P., *J. Phys. C*, 1982, **15**, 6361 (*theory*)

Stirlet, J.C. *et al*, *J. Less-Common Met.*, 1983, **92**, 227 (*use*)
Kirby, H.W., *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, 129 (*rev*)

IC-002795

[CPr]

Praseodymium carbides

Known phases include Pr_2C_3, PrC_2.

Praseodymium carbide ***(PrC_2)*** [12071-25-9]

C_2Pr M 164.9

Possesses CaC_2 struct. Brassy yellow cryst. Mp 2535°. $\mu_{eff} = 3.15\mu_B$ ($\theta = +5.2°$). Antiferromagnetic (T_N 7K). Undergoes transition from α to β form at 1130° (1100°). Dec. by H_2O affording principally C_2H_2 with lesser amounts of C_2H_4, C_2H_6 and other hydrocarbons.

Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1958, 498, 503, 505 (*synth, magnetism*)
Atoji, M. *et al*, *J. Chem. Phys.*, 1967, **46**, 1891 (*struct, magnetism*)
Anderson, J.S. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 105 (*reaction*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Sakai, T. *et al*, *J. Chem. Phys.*, 1981, **75**, 3027 (*magnetism*)

IC-002796

[CPu]

Plutonium carbides

[11116-02-2]

PuC_3, PuC_6, PuC_7, PuC_8 recently detected by ms; other main phases descr. here.

Plutonium carbide ***(Pu_3C_2)*** [12122-59-7]

C_2Pu_3 M 741.1

Obt. by annealing of arc-melted sample with 40 at. % C at 500°.

Plutonium carbide ***(PuC)***

Plutonium monocarbide

CPu M 251.0

Substoichiometric: PuC_{1-x}, usually approx. $PuC_{0.85}$, fcc struct. Synth. by arc melting of Pu-graphite mixtures in inert gas at 500°. Black solid. Attacked by hot H_2O. Mp 1654° (peritectic). Undergoes ferromagnetic ordering at 120K.

Plutonium carbide ***(Pu_2C_3)*** [12076-56-1]

Plutonium sequicarbide

C_3Pu_2 M 514.1

Bcc struct. in which all C present as C_2 groups. Synth. by carbothermic redn. of PuO_2 or from PuH_2 and C_3H_8 at 650-750°. Dull black solid. Mp 2050° (peritectic). ΔH_f° −83 kJ mol^{-1}.

Plutonium carbide ***(PuC_2)*** [12071-26-0]

C_2Pu M 263.0

Stable between ~ 1660 and 2230°. Has the CaC_2 struct. α- and β-forms exist. α-form is tetragonal, isomorphous with α-UC_2, β-form is cubic and stable above 1700°. Obt. by sintering of Pu_2C_3 with C at >1660°. Mp ~2250° (peritectic). Dec. to Pu_2C_3 + C <1750°.

[12075-34-2, 12076-55-0, 81858-75-5, 126214-37-7, 126214-38-8, 126214-39-9, 126214-40-2]

Kruger, O.L., *J. Am. Ceram. Soc.*, 1963, **46**, 80 (*synth*)
Rosen, S. *et al*, *J. Nucl. Mater.*, 1963, **10**, 90 (*synth, Pu_2C_3*)
Johnston, C.P. *et al*, *Prep. and Props. of Plutonium Carbide, A Bibliography*, 1963, MLM-1169 (*rev*)
Reshetnikov, F.G. *et al*, *At. Energ.*, 1967, **22**, 445 (*synth, PuC*)
Harper, E.A. *et al*, *Nature (London)*, 1968, **219**, 151 (*struct, PuC_2, Pu_2C_3*)
Battles, J.E. *et al*, *High Temp. Sci.*, 1970, **2**, 80 (*ms*)
Green, J.L. *et al*, *J. Nucl. Mater.*, 1970, **34**, 281 (*magnetism, nd*)
Alekseeva, Z.M. *et al*, *CA*, 1972, **76**, 145514z (*Pu_2C_3, PuC, Pu_2C_3, PuC_2 phases*)

Sheth, A. *et al*, *CA*, 1973, **83**, 67336 (*phys props, PuC*)
Johnson, G.K. *et al*, *J. Chem. Thermodyn.*, 1974, **6**, 219 (*thermodyn Pu_2C_3*)
Suzuki, Y. *et al*, *J. Nucl. Mater.*, 1981, **101**, 200 (*synth, Pu_2C_3*)
The Chemistry of the Actinide Elements, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, **1**, 667 (*rev*)
Datta, B.P. *et al*, *Int. J. Mass Spectrom. Ion Processes*, 1989, **91**, 241 (*ms, PuC_5, PuC_6, PuC_7, PuC_8*)

CRe

IC-002797

Rhenium carbide (ReC), 9CI

[12601-94-4]

ReC

M 198.2

Cubic-form

Fcc phase which dec. during annealing at 1000°. Synth. from Re and C at pressures 1.4×10^5 atm. and 1000°. Superconducting critical transition temp. at approx. 3.4 K.

Hexagonal-form

Hexagonal phase of the γ'-MoC kind. Synth. from Re and C at pressures up to 1.8×10^5 atm. and 1300°. Metastable at 1 atm. and dec. on annealing at 1000° to give a Re—C solid soln. Superconducting critical transition temp. at 1.6 K.

[11120-52-8]

Popova, S.V. *et al*, *High Temp. High Pressures*, 1971, **3**, 237.
Popova, S.V. *et al*, *Pis'ma Zh. Eksp. Teor. Fiz.*, 1972, **16**, 609; *CA*, **78**, 77134q.
Popova, S.V. *et al*, *Issled. Primen. Splavov Reniya, [Dokl. Vses. Soveshch. Probl. Reniya], 4th, 1973*, Ed., Savitskii, E.M., *et al*, 'Nauka', Moscow, 1975, 59; *CA*, **84**, 98640n.

[CReU]

IC-002798

Rhenium uranium carbides

Rhenium uranium carbide ***($Re_3U_3C_8$)*** [62712-26-9]

$C_8Re_3U_3$ M 1844.8

Alloy, tetragonal. Isol. from the Re—U—C phase system.

Rhenium uranium carbide ***($ReUC_2$)*** [12122-60-0]

C_2ReU M 448.2

Monoclinic phase which may be C-deficient. Isol. from the U—Re—C phase system.

[62700-36-1]

Alekseeva, Z.M. *et al*, *Kristallokhim. Intermet. Soedin., 2nd.*, Ed., Rylchal, R.M., L'vov. Gos. Univ., Lvov, USSR, 1974, 34; *CA*, **86**, 49287p.
Haines, H.R. *et al*, *Plutonium Other Actinides, Proc. Int. Conf., 5th, 1975*, Ed. Blenk, H, *et al*, North-Holland, Amsterdam, 1976, 233.
Alekseeva, Z.M. *et al*, *J. Nucl. Mater.*, 1977, **64**, 303 (*synth, struct*)

CRu

IC-002799

Ruthenium carbide (RuC)

[12012-13-4]

RuC

M 113.0

Isomorphous with WC in solid state, diatomic gas phase sp. Prepd. by the high temp. reaction between the elements. Exists in two phases. *D* (RuC) 644 kJ mol^{-1}.

[56126-84-2]

Kempter, C.P. *et al*, *J. Chem. Phys.*, 1960, **33**, 1580 (*solid-state*)
Nadler, M.R. *et al*, *J. Chem. Phys.*, 1960, **64**, 1468 (*synth*)
Kempter, C.P., *J. Chem. Phys.*, 1964, **41**, 1515 (*solid-state*)
Jeantet, B. *et al*, *Planseeber. Pulvermet.*, 1964, **12**, 12 (*synth*)

McIntyre, N.S. *et al*, *Trans. Faraday Soc.*, 1968, **64**, 3006 (*gas phase thermodyn*)
Gingerich, K.A., *Chem. Phys. Lett.*, 1974, **25**, 523 (*gas-phase thermodyn*)

IC-002800

CS

Carbon monosulfide

[2944-05-0]

CS

M 44.0

Obs. in upper atmosphere. Short-lived, highly-reactive gas. Rapidly forms brown-black polymer.

▷ Condensed CS polymerises explosively.

Klabunde, K.J. *et al*, *Inorg. Chem.*, 1974, **13**, 1778 (*synth, bibl*)
Klabunde, K.J. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 263.
Moltzen, E.K. *et al*, *Acta Chem. Scand., Ser. B*, 1986, **40**, 609 (*synth*)
Moltzen, E.K. *et al*, *J. Org. Chem.*, 1987, **52**, 1156 (*synth, bibl*)
Moltzen, G.K. *et al*, *Chem. Rev.*, 1988, **88**, 391 (*rev*)

IC-002801

CSSe

Carbon selenide sulfide, 9CI

Thiocarbonyl selenide. Carbon thioselenide

[5951-19-9]

S=C=Se ($C_{\infty v}$)

M 123.0

Interatomic distances: C—S 155.3, C—Se 169.3 pm. Synth. from FeSe + CS_2 at 650°. White solid at −190°; yellow liq. at 20°. Sol. org. solvs. Bp 83.9°, Bp 80-83°.

Briscoll, H.V.A. *et al*, *J. Chem. Soc.*, 1929, **59**, 1049 (*synth*)
Hirose, C. *et al*, *J. Chem. Phys.*, 1971, **55**, 5120 (*struct*)
Werner, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1979, **18**, 865 (*use*)
Henriken, L., *Synthesis*, 1985, 204 (*synth, nmr, cmr, bibl*)

[CSTi]

IC-002802

Titanium carbide sulfides

[39318-17-7]

Titanium carbide sulfide ***($TiCS_2$), 11CI*** [102790-27-2]

CS_2Ti M 124.0

Manuf. by ion implantation with S then with C into Ti. Cathode active material in alkaline batteries.

Titanium carbide sulfide ***($Ti_4C_2S_2$), 11CI*** [12542-08-4]

$C_2S_2Ti_4$ M 279.6

Struct. similar to TiP. Formed in Cr, Ti stainless steels or when Ti is added to a sulfur containing steel.

Narita, K. *et al*, *Tetsu To Hagane*, 1972, **58**, 1330; *CA*, **77**, 104386m (*cryst struct, $Ti_4C_2S_2$*)
Bold, T. *et al*, *Arch. Hutn.*, 1981, **26**, 289; *CA*, **96**, 166480p (*$Ti_4C_2S_2$ in steel*)
Nishikawa, S. *et al*, *Imono.*, 1981, **53**, 659; *CA*, **96**, 185136x (*$Ti_4C_2S_2$ in steel*)
U.S. Pat., 4 576 697, (1986); *CA*, **105**, 9278r (*manuf, use, $TiCS_2$*)

CS_2

IC-002803

Carbon disulfide

Carbon sulfide (CS_2). Carbon bisulfide. Dithiocarbonic anhydride

[75-15-0]

S=C=S ($D_{\infty h}$)

M 76.1

C–S 155.3 pm. Has disinfectant and insecticidal props.; used in manuf. of rayon and CCl_4, electronic vacuum tubes, org. solv. for sulphur, phosphorus, iodine, bromine, rubber intermediates, etc. Fumigation insecticide. Reagent in heterocyclic synth. Reagent for the gc and ms anal. of amines as isothiocyanates and for the anal. of thiols. Highly refracting colourless liq. Misc. EtOH, Et_2O, C_6H_6; spar. sol. H_2O. d_4^0 1.293. Mp −111.6°. Bp 46.5°, Bp_{297} 20°. n_D^{15} 1.6315. Forms hemihydrate, dec. at −3°. A black solid form has been prepd. at high press.

▷ Highly toxic by inhalation, TLV 30. Extremely flammable, flash p. −30°. FF6650000.

Bushell, W.J., *Chem. Ind. (London)*, 1961, 1465 (*rev*)
Namasimhachari, N. *et al*, *Anal. Biochem.*, 1972, **45**, 154 (*use*)
Jungen, C. *et al*, *Can. J. Phys.*, 1973, **51**, 1471 (*struct*)
Blanquet, G. *et al*, *Ann. Soc. Sci. Bruxelles*, 1974, **88**, 87 (*struct*)
Namasimhachari, N. *et al*, *Biomed. Mass Spectrom.*, 1974, **1**, 367 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 94.
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 742 (*rev*)
Verma, B.C. *et al*, *Mikrochim. Acta*, 1982, **1**, 393 (*use*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 6506.
Dunn, A.D. *et al*, *Carbon Disulphide in Organic Chemistry*, Ellis Horwood, 1989 (*rev*)
Tominaga, Y., *J. Heterocycl. Chem.*, 1989, **26**, 1167 (*rev, use*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 229.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 711.

CS_2V

IC-002804

Vanadium carbide sulfide (VCS_2), 11CI

[102790-28-3]

VCS_2

M 127.0

Formed on a V surface by successive ion implantation by S then C. Layers 1×10^5 - 2×10^5 pm deep are formed. Important as a cathode in non-aq. alkali metal batteries.

U.S. Pat., 4 576 697, (1986); *CA*, **105**, 9278r (*formn*)

CS_3Tl_2

IC-002805

Thallium(*I*) trithiocarbonate

$Tl_2(CS_3)$

M 516.9

Synth. from aq. $Tl^{\oplus}$ soln. and $Na_2CS_3.2H_2O$. Orange-red solid. Sol. H_2O (0.001 g per 100 cm^3), many polar and non-polar solvs. Dec. on heating to Tl_2S, CS_2, reacts with oxid. agents but stable to aq. alkalis and org. acids.

▷ Toxic.

Ingram, G., *J. Chem. Soc.*, 1957, 4328 (*synth, reactions*)
Krebs, B. *et al*, *Z. Naturforsch., B*, 1965, **20**, 1017 (*ir*)

IC-002806

[CSc]

Scandium carbides

Scandium carbide ***(ScC)*** [12012-14-5]

CSc M 56.9

Catalyses *ortho/para* conversion of H_2. Grey-black solid. Forms mainly CH_4 on hydrol.

Scandium carbide ***(Sc_3C_4)***

C_4Sc_3 M 182.9

Metallic conductor. Moisture-sensitive light grey lustrous cryst. (black powder). Originally reported as $Sc_{15}C_{19}$. First carbide found to contain C_3 units. On hydrol. affords a mixture of C_{1-3} hydrocarbons.

***Scandium carbide* (ScC_2)** [12175-91-6]
C_2Sc M 68.9
Water-sensitive solid. On hydrol. affords ethyne etc.
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 505 (*synth, ScC*)
Hajek, B. *et al*, *Monatsh. Chem.*, 1971, **102**, 1387 (*synth, ScC_2*)
Hque, R. *et al*, *J. Chem. Phys.*, 1981, **74**, 6407 (*ms*)
McColm, I.J., *J. Less-Common Met.*, 1981, **78**, 287 (*ScC_2*)
Hajek, B. *et al*, *J. Less-Common Met.*, 1984, **96**, 35 (*synth, C_4Sc_3*)
Pottgen, R. *et al*, *Inorg. Chem.*, 1991, **30**, 427 (*synth, cryst struct, C_4Sc_3*)

IC-002807

CSe_2

Carbon diselenide
Carbon selenide (CSe_2), 11CI, 9CI
[506-80-9]

Se=C=Se

M 169.9
Synth. from Se + CH_2Cl_2 at 500°. Malodorous photosensitive golden-yellow liq. V. sol. org. solvs; insol. H_2O. Mp −45°. Bp 125-126°, Bp_{50} 45.5-46°. Polymerises slowly at r.t. or on heating at 100° to an insol. black solid.

▷ Toxic.

Ives, D.J.G. *et al*, *J. Chem. Soc.*, 1947, 1080 (*synth*)
Gattow, G. *et al*, *Z. Anorg. Allg. Chem.*, 1966, **343**, 11 (*synth, uv, ir*)
Jensen, K.A., *Q. Rep. Sulfur Chem.*, 1970, **5**, 45 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 627 (*synth*)
Inorg. Synth., 1982, **21**, 6 (*synth*)
Okamoto, Y. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 386 (*props*)
Gombler, W. *et al*, *Z. Naturforsch., B*, 1982, **36**, 1561 (*cmr*)
Kobayashi, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 3821 (*polymers*)

IC-002808

CSi

Silicon(*IV*) carbide (SiC)
Carborundum
[409-21-2]

SiC

M 40.0
At least 70 modifications known, based on ZnS-type structs., α-form has wurtzite struct., β-form zinc blende struct. Commercially available abrasive powder. Refractory. When doped α-SiC is a valuable extrinsic semiconductor. Black, hexagonal or cubic cryst; colourless when pure. Insol. H_2O, acids; sol. fused KOH. Subl. ~2700° dec. Hardness: 9.5 Mohs.

▷ VW0450000.

Yajima, S. *et al*, *J. Mater. Sci.*, 1981, **16**, 1349 (*synth, cryst struct*)
Inoue, Z. *et al*, *J. Mater. Sci.*, 1982, **17**, 3197 (*synth, cryst struct*)
Finlay, G.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 159 (*Si-29 nmr*)
Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1986, 386 (*rev*)

IC-002809

[CSm]

Samarium carbides
Phases Sm_3C, Sm_2C_3, SmC_2 reported.
***Samarium carbide* (SmC_2)** [12071-28-2]
C_2Sm M 174.3
Possesses CaC_2 struct., probably $Sm^{3\oplus}(C_2^{\ominus})e^{\ominus}$. Yellow solid. Antiferromagnetic below 21K. Dec. by H_2O. α→β transition 1170°. ΔH_f° −96.2 kJ mol^{-1}. More volatile *in vacuo* than other Ln carbides.
Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, magnetism*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Sakai, T. *et al*, *J. Chem. Phys.*, 1981, **25**, 3027.
Haschke, J.M. *et al*, *J. Chem. Thermodyn.*, 1982, **14**, 1619 (*thermodyn data*)

IC-002810

[CTa]

Tantalum carbides
[51680-51-4]
A number a phases are known of which TaC and Ta_2C are the most important. Does not react with H_2O.
Tantalum carbide* (Ta_2C), *11CI [12070-07-4]
CTa_2 M 373.9
anti-CdI_2 struct. Synth. by arc-melting the components.
***Tantalum carbide* (Ta_4C_3)** [12076-61-8]
C_3Ta_4 M 759.8
Close packed Ta layers in 12-layer sequence with uncertain distribution of C. Synth. by reducing a $TaCl_5$/Ar vapour on graphite at 2000-2500°.
Tantalum carbide* (*TaC*), *11CI [12070-06-3]
CTa M 192.9
NaCl struct. Synth. from the elements, or by heating Ta in HCN or by electrolysis of an $Na_2B_4O_7/Na_2CO_3/NaF/KF/Ta_2O_5$ melt at 700° with a graphite cathode. Used in cutting tools, in the formulation of ceramics and cermets and a number of catalytic processes. Not hydrol.; v. hard.
Kebler, R.W., *NASA Tech. Rep.*, 1965, No. AD468830 (*synth, purif, TaC*)
Yvon, K. *et al*, *Acta Crystallogr., Sect. B*, 1970, **26**, 149 (*cryst struct, Ta_4C_3*)
Caillet, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **270**, 1867 (*synth, TaC*)
Terao, N., *Jpn. J. Appl. Phys.*, 1970, **9**, 1263 (*cryst struct, TaC*)
Hochman, A.J. *et al*, *J. Electrochem. Soc.*, 1983, **130**, 221 (*electrochem, synth, TaO*)
Demyashev, G.M. *et al*, *Izv. Akad. Nauk SSSR, Ser. Fiz.*, 1984, **48**, 1693 (*synth, Ta_4C_3*)
Loennberg, B. *et al*, *J. Less-Common Met.*, 1986, **120**, 239 (*synth, cryst struct, Ta_2C*)

IC-002811

[CTb]

Terbium carbides
Phases known include Tb_3C, Tb_2C_3, TbC_2.
***Terbium carbide* (TbC_2)** [12071-30-6]
C_2Tb M 182.9
CaC_2 struct. Brassy yellow powder. Undergoes α→β transition 1285°. $\mu_{eff} = 9.57\mu_B$ (θ −91.2°). Dec. by H_2O.
Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al*, *J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, magnetism*)
Atoji, M., *J. Chem. Phys.*, 1961, **35**, 1950; 1967, **46**, 1891 (*struct*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Sakai, T. *et al*, *J. Less-Common Met.*, 1981, **81**, 91 (*magnetism*)

[CTh]

Thorium carbides IC-002812
***Thorium carbide* (*ThC*)** [12012-16-7]
CTh M 244.0
Stoichiometry variable. Has NaCl type struct. with isolated C atoms. Moisture-sensitive solid. Mp 2625°. On hydrol. affords largely CH_4.
***Thorium carbide* (Th_2C_3)** [12151-76-7]
C_3Th_2 M 500.1
Synth. from Th + C at high pressure at 1200°. Moisture-sensitive solid. Superconductor below 4.1K. Studied as solid soln. with yttrium carbide.
***Thorium carbide* (ThC_2)** [12071-31-7]
C_2Th M 256.0
Exists in three cryst. forms: α (monoclinic) at r.t., β (bodycentred tetragonal) at 1430-1480°, γ (fcc) above 1480°. Cryst. forms differ in orientation of C_2 groups - fixed in α-form, disordered in 2D in β-form, 3D disordered in γ-form. Studied as fuel for fast breeder reactors. Moisture-sensitive yellow solid. Mp 2655°. Bp *ca.* 5000°. Dec. by H_2O. On hydrol. affords mainly C_2H_2, C_2H_6 + H_2.
Imai, H. *et al*, *J. Am. Ceram. Soc.*, 1967, **50**, 308 (*synth*)
Farkas, M.S., *ACS Symp. Ser.*, 1968, **12**, 445 (*use*)
Bowman, A.L. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 1121 (*cryst struct*)
Benz, R. *et al*, *High Temp. Sci.*, 1969, **1**, 114 (*phase diagram*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **5**, 357 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1158 (*synths*)
Olsen, J.S. *et al*, *Physica B+C (Amsterdam)*, B+C, 1980, **139-140**, 308 (*struct*)
Troost, L., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1983, **116**, 1229.
Katzin, L.I. *et al*, *The Chemistry of the Actinide Elements*, (Eds. Katz, J.J. *et al*), Chapman and Hall, London, 1986, 56 (*rev*)

IC-002813

CTi

Titanium carbide (TiC), 11CI
[12070-08-5]

TiC

M 59.8
At least 17 phases have been reported but only TiC has been studied in detail. TiC has an homogeneity range down to at least $Ti_{0.76}C$. Has the NaCl struct. which is retained in non-stoichiometric phases. There is an order⇌disorder transition at 760-790°. Synth. and manuf. involve reactions of Ti and C usually at high temps. eg. Ti + C black at 1800-2500°. Has a wide range of uses from abrasives and cutting tools to ceramics and anodes for Al refining. Mp 3137°.
[56780-56-4]
Christensen, A.N., *Acta Chem. Scand., Ser. A*, 1975, **29**, 563 (*cryst struct*)
Kato, A. *et al*, *Mem. Fac. Eng., Kyushu Univ.*, 1981, **41**, 319 (*synth, fine powder*)
Binder, F. *et al*, *Radex Rundsch.*, 1981, 690 (*manuf*)
Moisy-Maurice, V. *et al*, *Sci. Hard Mater.*, [*Proc. Int. Conf.*], *1981*, 1981, 83 (*order/disorder transition*)
Bonfiglioni, A. *et al*, *Metall. Ital.*, 1983, **75**, 259 (*rev, use*)
Kiparisov, S.S. *et al*, *Poroshk. Metall. (Kiev)*, 1983, 24; *CA*, **104**, 159784w (*manuf*)
Inzenhofer, A., *Fachber.*, 1984, **61**, 105 (*rev, use*)
Japan. Pat., 59 16 968, (1984); *CA*, **100**, 214501w (*manuf*)

[CTm]

Thulium carbides IC-002814
Phases known include Tm_3C, $Tm_{15}C_{19}$, TmC_2.
***Thalium carbide* (TmC_2)** [12180-16-4]
C_2Tm M 192.9
Possesses CaC_2 struct. Dec. by H_2O, mainly to C_2H_2. Undergoes α→β transition at 1355°. $\mu_{eff} = 7.2\mu_B$.
Spedding, F.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Anderson, J.S. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 105 (*hydrol*)
Atoji, M., *J. Chem. Phys.*, 1970, **52**, 6431 (*cryst struct, magnetism*)
Adachi, G. *et al*, *J. Less-Common Met.*, 1973, **32**, 301 (*struct*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Bauer, J. *et al*, *J. Less-Common Met.*, 1985, **109**, L9 (*synth*)

IC-002815

[CU]

Uranium carbides
[12612-73-6]
Three main phases, UC, U_2C_3, UC_3 known. U/Pu/C mixtures are potential fast breeder fuels.
▷ All three phases become pyrophoric when powdered.
***Uranium carbide* (*UC*)** [12070-09-6]
CU M 250.0
Possesses the NaCl struct. Reactor fuel of high potential owing to high fissionable material density and good conductivity. Bright grey black solid with metallic shine. Mp 2500°. Bp *ca.* 4400° (extrap.). On hydrol. affords largely CH_4 + other alkanes. Metallic conductor. Paramagnetic (below r.t. virtually temp. independent).
***Uranium carbide* (U_2C_3)** [12076-62-9]
C_3U_2 M 512.0
Isostructural with Pu_2C_3. Synth. by UC/UC_2 fusion at 1200-1800°: cannot be obt. by direct U-C fusion. Black solid with metallic lustre. Affords various alkanes on hydrol. Antiferromagnetic at low temps. (T_N = 57-59°) Curie-Weiss behaviour between 70-550K.
***Uranium carbide* (UC_2)** [12071-33-9]
C_2U M 262.0
Exists in α and β-forms. α-form has CaC_2 struct. β-form stable >1770° has KCN struct. Paramagnetic to 0K (near-temp. independent). Light grey metallic cryst. Dec. by H_2O. Mp 2500°. Bp 4370°. At 700° with H_2→UC + CH_4. On hydrol. forms CH_4, C_2H_6, H_2 + other hydrocarbons.
Lebeau, P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1913, **156**, 1987 (*synth, hydrol*)
Rundle, R.E. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 99 (*cryst struct*)
Litz, L.M. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 1718 (*cryst struct*)
Mallet, M.W. *et al*, *J. Electrochem. Soc.*, 1951, **98**, 508; 1952, **99**, 197 (*synth, cryst struct*)
Atoji, M. *et al*, *J. Chem. Phys.*, 1959, **31**, 332 (*struct, U_2C_3*)
Bradley, M.J. *et al*, *Inorg. Chem.*, 1962, **1**, 683; 1964, **3**, 189 (*hydrol*)
Bates, L.F. *et al*, *Brit. J. Appl. Phys.*, 1964, **15**, 543 (*magnetism, UC*)
de Norian, C.H. *et al*, *Phys. Lett.*, 1965, **19**, 455 (*magnetism, U_2C_3*)
Browian, A.L. *et al*, *Acta Crystallogr.*, 1966, **21**, 670 (*cryst struct*)
Harper, E.A. *et al*, *Nature (London)*, 1968, **219**, 151 (*struct*)
Raphael, G. *et al*, *Solid State Commun.*, 1969, **7**, 791 (*magnetism, U_2C_3*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1240 (*synth*)
Weinberger, P. *et al*, *J. Phys. C*, 1979, **12**, 801 (*electronic struct, UC*)
Brooks, M.S.S., *J. Phys. F*, 1984, **14**, 639 (*electronic struct, UC*)
Gmelin Handbook Inorg. Chem., Syst. No. 55, Suppl. Vol., 1987, **C12**, 1 (*rev, UC*)

[CV] IC-002816

Vanadium carbides

[11130-21-5]

Two well-characterised phases are known and at least 14 others. Most work has been done with components in alloys rather than with single substances. The major importance of these compds. is in their formation in alloy steels and in ceramics.

Vanadium carbide (V_2C) [12012-17-5]

CV_2 M 113.8

Struct. comprises hcp V with C in octahedral sites in an ordered defect struct. (ε—Fe_2N struct.). V_6C_5 and V_8C_7 are also ordered defect structs. based on an NaCl lattice. Synth. by heating the elements or manuf. by heating $VO(OH)_2$ and C under Ar in an induction furnace.

Vanadium carbide (V_4C_3), ***9CI*** [12076-63-0]

C_3V_4 M 239.7

12 Layer close packed V metal struct. with C disordered amongst O_h sites. Synth. by hot pressing V + C in graphite dies.

Vanadium carbide (V_6C_5), ***9CI*** [12181-74-7]

C_5V_6 M 491.6

NaCl struct. with perfect spiral array of defects on the C sub-lattice. Synth. by heating pellets of V + C for 100 h at 1650°.

Vanadium carbide (*VC*) [12070-10-9]

CV M 62.9

NaCl-type struct. Synth. from V_2O_5 and C in an Ar plasma or by heating ferrovanadium, V and C black to 1700-2000° in a vacuum induction furnace. Not hydrol. unlike most interstitial carbides.

Rudy, E. *et al. J. Am. Ceram. Soc.*, 1967, **50**, 265 (*cryst struct, V_2C*)
Yvon, K. *et al. Acta Crystallogr., Sect. B*, 1970, **26**, 149 (*synth, cryst struct, V_4C_3*)
Henfrey, A.W. *et al. Acta Crystallogr., Sect. B*, 1970, **26**, 1882 (*synth, rel, V_4C_3*)
Terao, N., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **275**, 1165 (*synth, cryst struct, V_2C*)
Lewis, M.H., *Philos. Mag.*, 1975, **31**, 173 (*cryst struct, VC*)
Marx, F. *et al. Rev. Roum. Chim.*, 1978, **23**, 417; *CA*, **88**, 196264y (*synth, VC*)
Belg. Pat., 886 836, (1981); *CA*, **95**, 171967m (*manuf, V_2C*)
Binder, F. *et al. Radex Rundsch.*, 1981, 680; *CA*, **96**, 204273h (*manuf, VC*)

[CW] IC-002817

Tungsten carbides

[11130-73-7]

Tungsten carbide (W_2C), ***9CI*** [12070-13-2]

CW_2 M 379.7

Exists in two allotropic forms. (i) hexagonal, stable up to 2000° (ii) ccp with NaCl struct. Synth. by sintering stoichiometric amounts of W and C. Commercially available. Black cryst. with a hardness approaching that of diamond. Mp 2860°. Various substoichiometric phases known for W_2C_n where $0.76 \leqslant n \leqslant 1$.

Tungsten carbide (*WC*) [12070-12-1]

CW M 195.8

Layer struct. with alternating W and C with metal metal bonds within layers. Synth. e.g. by heating finely divided W + carbon to *ca.* 2200°. Commercially available. Most important phase in cemented carbides, crucibles, dyes, furnace parts etc. Approx. 15,000-18,000 metric tons produced annually. Solid with metallic lustre. Electrical conductor. Insol. Mp >2755° dec. Various compositions known for WC_n where $0.41 \leqslant n \leqslant 1$.

▷ YO7250000.

Becker, K. *et al. Z. Angew. Chem.*, 1927, **40**, 512 (*synth, W_2C*)
Leciejewicz, J., *Acta Crystallogr.*, 1961, **14**, 200 (*struct, WC*)
Lautz, Von G. *et al. Z. Naturforsch., A*, 1961, **16**, 1368 (*WC, W_2C struct*)
Goldschmidt, H.J. *et al. J. Less-Common Met.*, 1963, **5**, 181 (*synth, W_2C*)
Yvon, K. *et al. Monatsh. Chem.*, 1968, **99**, 726 (*W_2C, cryst struct*)
Storms, E.K., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. One*, 1972, **10**, 37 (*phases, phys progs*)
Muddock, A.G. *et al. J. Chem. Soc., Dalton Trans.*, 1974, 1314 (*W_2C, mössbauer*)
Harsta, A. *et al. Acta Chem. Scand., Ser. A*, 1978, **32**, 891 (*struct, rel, W_2C*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **4**, 491 (*rev*)
Demyashev, G.M. *et al. Izv. Akad. Nauk SSSR Neorg. Mat.*, 1985, **21**, 1155 (*struct, W_4C*)

[CY] IC-002818

Yttrium carbides

Yttrium carbide (YC_2) [12071-35-1]

C_2Y M 112.9

Possesses CaC_2 struct. Catalyst for hydrogenation of acetylenes. Used to make conductive ceramics. Yellow microcryst. Mp 2145°. Dec. by H_2O, largely to ethylene. $\alpha \rightarrow \beta$ transition temp. 1320°.

Spedding, F.H. *et al. J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al. J. Chem. Soc.*, 1959, 498, 505 (*synth*)
Atoji, M., *J. Chem. Phys.*, 1961, **35**, 1950 (*struct*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Male, G., *Rev. Int. Hautes Temp. Refract.*, 1977, **14**, 179 (*synth*)
Hajek, B. *et al. Collect. Czech. Chem. Commun.*, 1984, **49**, 936, 944 (*synth, hydrol*)
Jones, D.W. *et al. J. Solid State Chem.*, 1984, **53**, 376 (*struct*)
Japan. Pat., 60 51 661, (1985); *CA*, **103**, 41442 (*use*)
McKee, D.W., *Carbon*, 1986, **24**, 331 (*use*)
Karen, P. *et al. Collect. Czech. Chem. Commun.*, 1986, **51**, 1411 (*hydrol*)

[CYb] IC-002819

Ytterbium carbides

Phases known include Yb_2C, YbC_2.

Ytterbium carbide (YbC_2) [12180-18-6]

C_2Yb M 197.0

Possesses CaC_2 struct. Yellow solid. On hydrol. affords principally C_2H_2, with some C_2H_4 and C_2H_6, as well as other hydrocarbons. $\mu_{eff} = 3.69\mu_B$ (θ −388°).

Spedding, F.H. *et al. J. Am. Chem. Soc.*, 1958, **80**, 4499 (*synth, struct*)
Vickery, R.C. *et al. J. Chem. Soc.*, 1959, 498, 503, 505 (*synth, struct*)
Atoji, M., *J. Chem. Phys.*, 1961, **35**, 1950 (*struct*)
Anderson, J.S. *et al. J. Inorg. Nucl. Chem.*, 1968, **30**, 105 (*hydrol*)
Adachi, G. *et al. J. Less-Common Met.*, 1973, **32**, 301 (*synth, struct*)
Potter, P.E., *MTP Int. Rev. Sci.: Inorg. Chem., Ser. Two*, 1975, **7**, 257 (*rev*)
Sales, B.C., *Proc. Int. Conf. Low Temp. Phys., 14th, 1975*, 1975, **3**, 487; *CA*, **85**, 55764 (*magnetism*)

[CZr] IC-002820

Zirconium carbides

[51680-56-9]

Several carbides have been reported but only ZrC has been extensively studied.

Zirconium carbide (Zr_2C), ***11CI*** [12179-95-2]

CZr_2 M 194.4

Defect NaCl struct. No evidence for ordering of defects in the stoichiometric phase. Synth. by heating Zr and C.

Zirconium carbide (ZrC), ***11CI*** [12070-14-3]

CZr M 103.2

NaCl struct. Manuf. by reducing $ZrSiO_4$ with C in an electric furnace. Synth. by condensing Zr vapour on graphite at 1700° or heating ZrO_2 and graphite to 2200° at 500 atm. Used chiefly in abrasives and cutting tools.

Suzuki, H. *et al. Bull. Tokyo Inst. Technol.*, 1963, **54**, 159 (*synth, ZrC*)
Samsonov, G.V. *et al. Monatsh. Chem.*, 1971, **102**, 1667 (*synth, ZrC*)
Gerl, L.M. *et al. Izv. Akad. Nauk SSSR Neorg. Mat.*, 1972, **8**, 351; *CA*, **76**, 118228c (*synth, ZrC*)
Ohata, N. *et al. J. Nucl. Mater.*, 1976, **60**, 39 (*cryst struct, Zr_2C*)
Japan. Pat., 80 51 713, (1980); *CA*, **93**, 97805a (*manuf, ZrC*)
Andrievskii, R.A., *Poroshk. Metall. (Kiev)*, 1982, 37; *CA*, **96**, 221075q (*rev, ZrC*)
Arbuzov, M.P. *et al. Dopov. Akad. Nauk Ukr. RSR, Ser. A: Fiz. Mat. Tekh. Nauki.*, 1983, 73; *CA*, **99**, 131648j (*synth, cryst struct, Zr_2C*)

$C_2AgN_2^{\ominus}$ IC-002821

Bis(cyano-*C*)argentate(1 −), 9CI

Dicyanoargentate(1 −)

[15391-88-5]

$[Ag(CN)_2]^{\ominus}$

M 159.9 (ion)

Linear anion.

Na salt: [21430-69-3].

White cryst. Sol. H_2O.

K salt: [506-61-6]. *Potassium silver cyanide*

C_2AgKN_2 M 199.0

Used in silver plating and as bactericide. White, light-sensitive cryst. Sol. H_2O.

▷ TT5775000.

Bunett, H. *et al. J. Chem. Soc.*, 1924, 1660 (*synth*)
Stanitzky, E., *Anal. Chem.*, 1956, **28**, 419 (*cryst struct*)
Chadwick, B.M. *et al. J. Mol. Struct.*, 1968, **2**, 281 (*raman, ir*)
Loehr, T.M. *et al. J. Chem. Phys.*, 1970, **53**, 4182 (*ir, raman*)
Mason, W.R. *et al. J. Am. Chem. Soc.*, 1973, **95**, 3573 (*uv*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, 1976, 272 (*rev*)
Merck Index, 11th Ed., 1989, No. 7659.

$C_2Ag_2O_4$ IC-002822

Silver(*I*) oxalate

Ethanedioic acid silver salt

[533-51-7]

$Ag_2(C_2O_4)$

M 303.7

Struct. consists of chains of $Ag_2C_2O_4$ units. Used in photographic emulsion. White, crystalline powder. V. spar. sol. H_2O. Sol. conc. HNO_3, NH_3. ΔH_f° −675.8 kJ mol^{-1}.

▷ Dec. violently at 140°. RO2900000.

Macdonald, J.Y., *J. Chem. Soc.*, 1936, 832 (*synth*)
Douville, F. *et al. Compt. Rend. Hebd. Seances Acad. Sci.*, 1941, **212**, 697 (*ir*)
Berton, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1941, **213**, 1001 (*uv*)
Griffith, R.L., *J. Chem. Phys.*, 1943, **11**, 499 (*cryst struct, synth*)
Finch, A. *et al. J. Chem. Soc.*, 1954, 2053 (*photochem*)
Szabó, Z.G. *et al. Z. Elektrochem.*, 1956, **60**, 869 (*synth, electrochem*)
Lega, A.G., *J. Phys. Chem.*, 1966, **70**, 3254 (*synth*)

Merck Index, 11th Ed., 1989, No. 8467
Sax, N.I. *et al. Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3052.

$C_2AuN_2^{\ominus}$ IC-002823

Bis(cyano-*C*)aurate(1 −), 10CI, 9CI

Dicyanoaurate(1 −)

[14950-87-9]

$[Au(CN)_2]^{\ominus}$

M 249.0 (ion)

Many salts known.

K salt: [13967-50-5]. *Gold potassium cyanide*

C_2AuKN_2 M 288.1

Colourless cryst. (H_2O), air and light stable. Sl. sol. H_2O; spar. sol. EtOH; insol. Et_2O, Me_2CO.

H compd.: [60625-20-3].

C_2HAuN_2 M 250.0

Colourless cryst. Ir ν_{CN} 2147 (soln.), 2212 cm^{-1} (solid). Dec. rapidly to AuCN at 120°.

Chemnitius, F., *Chem.-Ztg.*, 1927, **51**, 823 (*synth*)
Penneman, R.A. *et al. J. Am. Chem. Soc.*, 1956, **78**, 62 (*synth, ir*)
Rosenzweig, A. *et al. Acta Crystallogr.*, 1959, **12**, 709 (*cryst struct*)
Jones, D. *et al. Nature (London)*, 1962, **196**, 277
Jones, L.H., *Spectrochim. Acta*, 1963, **19**, 1675 (*ir*)
Evans, D.F. *et al. J. Chem. Soc.*, 1964, 3164 (*ir*)
Fultons, M.O. *et al. J. Chem. Phys.*, 1970, **53**, 4249 (*mössbauer*)
Bruzer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, 2, 1018 (*synth*)
Miller, B. *et al. J. Electrochem. Soc.*, 1976, **123**, 1006 (*conductivity*)
Pesek, J.J. *et al. Inorg. Chem.*, 1979, **18**, 924 (*raman*)

$C_2AuN_2O_2^{\ominus}$ IC-002824

Bis(fulminato-*C*)aurate(1 −), 10CI

Difulminatoaurate(I)

[30179-40-9]

$[ONC{-}Au{-}CNO]^{\ominus}$

M 281.0 (ion)

Ph_4As salt: Cryst. (Me_2CO aq.).

Beck, W. *et al. Chem. Ber.*, 1970, **103**, 3591 (*synth*)
Nagel, U. *et al. J. Organomet. Chem.*, 1980, **185**, 427 (*cryst struct*)

C_2AuO_2 IC-002825

Dicarbonylgold

Gold dicarbonyl

[60594-90-3]

$Au(CO)_2$

M 252.9

Prepd. by cocondensation of Au and CO in inert gas matrix. Stable to 70K. Ir ν_{CO} 1935.8 cm^{-1}.

McIntosh, D. *et al. Inorg. Chem.*, 1977, **16**, 51 (*synth, ir*)

C_2Au_2 IC-002826

Gold acetylide, 9CI

[70950-00-4]

$[Au{\equiv}CAu]_n$

M 417.9

Polymeric. Yellow powder. Insol. common org. solvs.

▷ Explosive on heating or mechanical impact especially when dry.

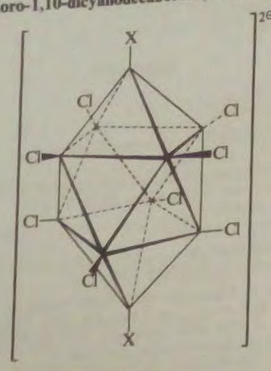
Mathews, A. *et al. J. Am. Chem. Soc.*, 1900, **22**, 108 (*synth, haz*)
Nast, R. *et al. Z. Anorg. Allg. Chem.*, 1964, **330**, 311.

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-81, **2**, 1063 (*synth*)
Nast, R., *Angew. Chem.*, 1965, **77**, 352 (*rev*)

IC-002827

$C_2B_{10}Cl_8N_2^{2\ominus}$

Octachloro-1,10-dicyanodecaborate(2−), 8Cl



X = CN

M 443.7 (ion)

Di-Cs salt:
$C_2B_{10}Cl_8Cs_2N_2$ M 709.5
Colourless cryst. (hot H_2O). Sol. H_2O, MeCN.

Bis-Me_4N salt: Colourless cryst. (aq. MeCN/EtOH). Sol. MeCN.

Trofimenko, S. *et al, J. Am. Chem. Soc.*, 1965, **87**, 653; 1966, **88**, 1899 (*synth, ir, B-11 nmr*)

IC-002828

$C_2B_{10}Cl_8N_2O_2^{2\ominus}$

Octachloro-1,10-bis(isocyanato)decaborate(2−), 8Cl

As Octachloro-1,10-dicyanodecaborate(2−), IC-002827 with

X = NCO

M 475.7 (ion)

closo-.

Bis-Me_4N salt: Colourless solid. Sol. MeCN; spar. sol. EtOH. Mp > 400°.

Knoth, W.H. *et al, J. Am. Chem. Soc.*, 1967, **89**, 4842 (*synth, uv*)
U.S. Pat., 3 390 966, (1968); *CA*, **69**, 44973 (*synth, uv, ir*)

IC-002829

C_2BaMgO_6

Barium magnesium carbonate ($BaMg(CO_3)_2$)

Magnesium barium carbonate. Carbonic acid, barium magnesium salt (2:1:1), 8CI

[52969-83-2]

$BaMg(CO_3)_2$

M 281.6

Synth. e.g. by reaction of the constit. carbonates at 500° and 15 × 10^3 atm. Colourless hexagonal cryst.

Mineral-form

Norsethite

Isotypic with calcite. Found in USA, USSR and Namibia. Clear to milky white circular plates or rhombohedral cryst.

Chang, L.L.Y., *Am. Mineral.*, 1964, **49**, 1142 (*synth*)
Hood, W.C. *et al, Am. Mineral.*, 1974, **59**, 471 (*synth*)
Effenberger, H. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1985, **171**, 275 (*cryst struct*)

IC-002830

$C_2BaN_2S_2$

Barium thiocyanate

Thiocyanuric acid, barium salt, 8CI

[2092-17-3]

$Ba(NCS)_2$

M 253.4

Prep. either by reaction of $[NH_4]SCN$ with $Ba(OH)_2.8H_2O$ or by slow neutralisation of $BaCO_3$ with aq. HSCN. Cryst. as trihydrate which gives anhydrous $Ba(SCN)_2$ on drying in air. Reagent for converting metal sulfates to thiocyanates. White solid, highly hygroscopic. V. sol. H_2O; sol. Me_2CO, MeOH, EtOH.

Dihydrate: [5908-82-7].
$C_2H_4BaN_2O_2S_2$ M 289.5
Incorrectly formulated; structural analysis has shown this species to be the trihydrate.

Trihydrate: [68016-36-4].
$C_2H_6BaN_2O_3S_2$ M 307.5
Commercially available. Colourless monoclinic cryst., deliquescent. Dec. on heating with H_2O loss. Sol. H_2O (4.3 g per 100cm^3 at 20°); v. sol. EtOH (35g per 100 cm^3 at 20°).

▷ Irritant.

Inorg. Synth., 1950, **3**, 24 (*synth*)
Zvonkova, Z.V. *et al, Zh. Fiz. Khim.*, 1950, **24**, 1345 (*dihydrate, original cryst struct*)
Tramer, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1961, **253**, 1679 (*hydrate, ir, raman*)
Tramer, A., *J. Chim. Phys. Phys.-Chim. Biol.*, 1962, **59**, 637 (*hydrate, ir, raman*)
Krasser, W. *et al, Naturwissenschaften*, 1967, **54**, 134 (*raman*)
Kargol, J.A. *et al, Inorg. Chem.*, 1979, **18**, 2532 (*cmr*)
Mereiter, K. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 382 (*trihydrate, revised cryst struct*)

IC-002831

C_2BaO_4

Barium oxalate (BaC_2O_4)

Ethanedioic acid, barium salt, 9CI. Oxalic acid, barium salt, 8CI

[516-02-9]

$Ba(C_2O_4)$

M 225.3

Synth. by reaction of $BaCl_2$ and either sodium oxalate or oxalic acid in aq. soln. Cryst. as dihydrate. Thermal dec. yields the anhydrous material. White powder. Dissolves in acids. Dec. on heating with $BaCO_3$ formn. Prac. insol. H_2O (0.0093 g per 100 cm^3 at 18°; 0.023 g per 100 cm^3 at 100°); insol. EtOH.

Hemihydrate: [18581-89-0].
Prepd. by partial dehydration of the dihydrate. Colourless cryst. Dec. on heating with H_2O loss.

Monohydrate: [13463-22-4].
Prepd. by partial dehydration of the dihydrate. Colourless monoclinic cryst. Dec. on heating with H_2O loss.

Dihydrate: [18581-91-4].
Cryst. from soln. formed by mixing aq. $BaCl_2$ with either aq. sodium oxalate or aq. oxalic acid. Colourless monoclinic cryst. Dec. on heating with H_2O loss to form the lower hydrates and then the anhydrous compd.

Gerard, N. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **265**, 1436 (*thermal dissoc, hydrates*)

Mutin, J.C., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1971, **273**, 1512; 1974, **278**, 1001 (*cryst structs, dihydrate, monohydrate*)
Fabbri, G. *et al, Atti. Soc. Nat. Mat. Modena*, 1975, **106**, 57, 81; *CA*, 1977, **86**, 182308, 182309 (*ir, thermal dec monohydrate*)
Derouane, E.G. *et al, Thermochim. Acta*, 1975, **11**, 287 (*thermal dec*)
Mutin, J.C. *et al, Colloq. Int. C.N.R.S.*, 1977, 1978, **277**, 123; *CA*, 1979, **90**, 178453 (*struct chem, hydrates*)
Mutin, J.C. *et al, J. Solid State Chem.*, 1981, **36**, 356 (*cryst struct, hemihydrate*)
Mu, J. *et al, Thermochim. Acta*, 1981, **49**, 207 (*thermal dec*)
Ben Amor, M. *et al, J. Solid State Chem.*, 1983, **48**, 231, 242 (*thermal dec, dihydrate, synth, monohydrate*)
Zaki, M.I. *et al, Thermochim. Acta*, 1984, **78**, 29 (*synth, props, hemihydrate*)
Bhatti, A.S. *et al, Thermochim. Acta*, 1984, **78**, 63 (*synth*)

IC-002832

$C_2BrF_6NO_4S_2$

***N*-Bromobis(trifluoromethylsulfonyl)imide**

N-Bromo-1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl] methanesulfonamide, 9CI. N-Bromoimidobis(trifluoromethyldisulfuryl) fluoride

[104715-39-1]

$BrN(SO_2CF_3)_2$

M 360.0

Synth. from $BrOSO_2F$ + $Hg[N(SO_2CF_3)_2]_2$ at 20°. Pale yellow liq.; stable in the dark. Mp −25°. Forms BrCl with AgCl.

Singh, S. *et al, Inorg. Chem.*, 1986, **25**, 4596 (*synth, ir, ms, F-19 nmr*)

IC-002833

C_2BrF_9NS

[Bromo[(trifluoromethyl)imino]methyl]pentafluorosulfur, 9CI

Bromo(pentafluorothio)-N-(trifluoromethyl)methanimine

[99298-44-9]

$F_3CN{=}C(Br)SF_5$

M 301.9

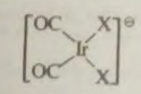
Only 1 isomer detected. Colourless liq. Bp 81°.

Lentz, D. *et al, Inorg. Chem.*, 1985, **24**, 4665 (*synth, ir, raman, ms, F-19 nmr*)

IC-002834

$C_2Br_2IrO_2^{\ominus}$

Dibromodicarbonyliridate(1−), 10CI



X = Br

M 408.0 (ion)

cis-form

Tetrabutylammonium salt: [73190-78-0].
Yellow needles (EtOH). Mp 92°.

Ph_4As salt: [30191-85-6].
Yellow cryst. (EtOH). Mp 228°. Ir ν_{CO} 2055, 1975 cm^{-1} ($MeNO_2$).

Malatesta, L. *et al, J. Inorg. Nucl. Chem.*, 1961, **19**, 81 (*synth, ir*)
Forster, D., *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 433 (*synth, ir*)
Cleare, M.J. *et al, J. Chem. Soc. A*, 1970, 2788 (*synth, ir*)
Pesano, P. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 1237 (*synth, ir*)

IC-002835

$C_2Br_2IrO_2$

Dibromodicarbonyliridium

$[Ir(CO)_2Br_2]_n$

M 408.0

Polymeric, *n* unknown. Pale-yellow cryst. Subl. 150° in a stream of CO.

Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1941, **246**, 138 (*synth*)

IC-002836

$C_2Br_2N_2Zr$

Zirconium bromide cyanide ($ZrBr_2(CN)_2$), 11CI

Zirconium dibromide dicyanide

[97458-81-6]

$ZrBr_2(CN)_2$

M 303.0

Synth. by dissolving $ZrBr_4$ and NH_4CN in liq. NH_3 and heating the solid product to 250° *in vacuo* to remove NH_4Br and NH_4CN. Brown solid.

Boyle, E.L. *et al, Inorg. Chim. Acta*, 1985, **100**, 281 (*synth, ir*)

IC-002837

$C_2Br_2O_2Pt$

Dibromodicarbonylplatinum, 10CI

Dibromoplatinum dicarbonyl. Dicarbonylplatinum dibromide

M 410.9

cis-form [20963-52-4]
More stable form. Cryst. Subl. 220° (under CO). Ir ν_{CO} 2162, 2119 cm^{-1} (toluene).

trans-form [106863-43-8]
Unstable: readily converts to cis even as solid. Cryst. (1,2-dichloroethane/heptane). Ir ν_{CO} 2136 cm^{-1} (toluene).

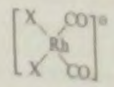
Browning, J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, raman, nmr*)
Caldrazzo, F. *et al, Pure Appl. Chem.*, 1986, **58**, 561 (*synth, ir*)
Andreini, B.P. *et al, J. Organomet. Chem.*, 1988, **354**, 357 (*ir, cmr, synth, props*)

IC-002838

$C_2Br_2O_2Rh^{\ominus}$

Dibromodicarbonylrhodate(1−), 10CI

[44516-32-7]



X = Br

M 318.7 (ion)

cis-form [44516-36-1]
Solns. become red when left in air owing to oxidn. to Rh(III) species.

Ph_4As salt: [30193-20-5].
Pale-yellow cryst. (Me_2CO/pet. ether). Mp 130° dec. Ir ν_{CO} 2055, 1975 cm^{-1} (nujol).

Tetrapropylammonium salt: [66197-28-2].
Yellow cryst. (CH_2Cl_2/Et_2O). Mp 104-108° dec. Ir ν_{CO} 2067, 1995 cm^{-1} (nujol).

Tetrabutylammonium salt: [30191-99-2].
Pale-yellow cryst. (Me_2CO/pet. ether). Mp 86° dec. Ir ν_{CO} 2062, 1985 cm^{-1} (nujol).

Vallarino, L.M., *Inorg. Chem.*, 1965, **4**, 161 (*synth, ir*)

Kingston, J.F., *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 65 (*synth, ir*)
Griffith, W.P. *et al, J. Chem. Soc. A*, 1970, 2788 (*synth, ir, raman*)
Geoffroy, G.L. *et al, Inorg. Chem.*, 1977, **16**, 1950 (*uv, mcd*)
Browning, J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, raman, cmr*)
Brown, C. *et al, J. Organomet. Chem.*, 1980, **192**, 93 (*nmr*)

IC-002839

$C_2Br_2O_2Ru$
Dibromodicarbonylruthenium, 9CI, 8CI
[16369-41-8]

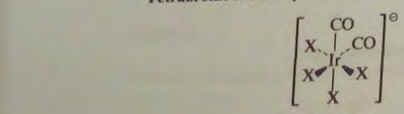
$Ru(CO)_2Br_2$

M 316.8
Monomeric and polymeric forms known.
Polymer: [28986-71-2].
Cream solid.

Colton, R. *et al, Aust. J. Chem.*, 1967, **20**, 1283 (*synth, ir*)
Sandhu, S.S. *et al, Indian J. Chem.*, 1972, **10**, 946.

IC-002840

$C_2Br_4IrO_2^{\ominus}$
Tetrabromodicarbonyliridate(1−), 10CI



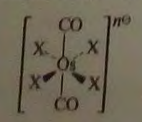
X = Br

M 567.8 (ion)
cis-form
K salt:
$C_2Br_4IrKO_2$ M 606.9
Yellow cryst.
Cs salt: [30191-97-0].
$C_2Br_4CsIrO_2$ M 700.7
Cryst.
Et_4N salt: [54032-04-1].
Shiny orange cryst.
Ph_4As salt: [30191-82-3].
Bright-yellow cryst. (Me_2CO). Ir ν_{CO} 2133, 2087 cm^{-1} ($CHCl_3$).

Malatesta, L. *et al, J. Inorg. Nucl. Chem.*, 1961, **19**, 81 (*synth, ir*)
Cleare, M.J. *et al, J. Chem. Soc. A*, 1970, 2788 (*synth, ir*)
Forster, D., *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 221 (*synth, ir*)
Forster, D., *Inorg. Chem.*, 1972, **11**, 473 (*synth*)
Malatesta, L., *J. Organomet. Chem.*, 1974, **73**, 265 (*synth, ir*)

IC-002841

$C_2Br_4O_2Os^{\ominus}$
Tetrabromodicarbonylosmate(1−), 9CI



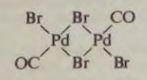
X = Br, *n* = 1

M 565.8 (ion)
trans-form
Tetrabutylammonium salt: [55399-52-5].
Dark-red needles (CH_2Cl_2). Sol. Me_2CO, $CHCl_3$, CH_2Cl_2, mod. sol. EtOH.

Preetz, W. *et al, J. Organomet. Chem.*, 1975, **86**, 397 (*synth, ir, uv*)

IC-002842

$C_2Br_4O_2Pd_2$
Di-μ-bromodibromodicarbonyldipalladium(*II*), 9CI
[21097-57-4]

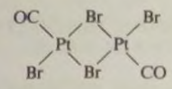


M 588.4
Catalyst for carboxylation of acetylene. Bright-yellow cryst. (H_2O). Orange cryst. (heptane). Ir ν_{CO} 2148 cm^{-1} (toluene). Best stored under CO atm.
Monomer:
CBr_2OPd M 294.2
Unknown.

Kutyukov, G.G. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 809 (*synth*)
Andreini, B.P. *et al, J. Organomet. Chem.*, 1988, **354**, 369 (*synth, ir, props*)

IC-002843

$C_2Br_4O_2Pt_2$
Di-μ-bromodibromodicarbonyldiplatinum(*II*)
Tetrabromodicarbonyldiplatinum
[106863-39-2]



M 765.7
Orange cryst. (hexane). Ir ν_{CO} 2119 cm^{-1} (toluene).

Calderazzo, F. *et al, Pure Appl. Chem.*, 1986, **58**, 561 (*synth, ir*)
Andreini, B.P. *et al, J. Organomet. Chem.*, 1988, **354**, 357 (*synth, ir, cmr*)

IC-002844

$C_2Br_4O_2Rh^{\ominus}$
Tetrabromodicarbonylrhodate(1−), 9CI

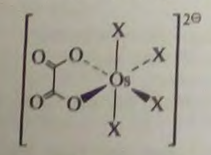
$[RhBr_4(CO)_2]^{\ominus}$

M 478.5 (ion)
Octahedral complex.
cis-form [24596-70-1]
Characterised spectroscopically. Ir ν_{CO} 2146, 2115 cm^{-1} ($CHCl_3$).
trans-form [55659-62-6]
Characterised spectroscopically.

Forster, D., *Inorg. Chem.*, 1969, **8**, 2556 (*synth, ir*)
Daly, J.J. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2551 (*synth*)

IC-002845

$C_2Br_4O_4Os^{2\ominus}$
Tetrabromo(oxalato)osmate(*IV*)(2−)
Tetrabromo[ethanedioato(2−)-O,O']osmate(2−), 10CI



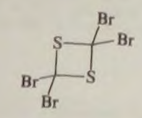
X = Br

M 597.8 (ion)
Synth. from oxalic acid and $K_2(OsBr_6)$.
Di-Cs salt: [74325-51-2].
Orange-red.
Bis-tetrabutylammonium salt: [74325-55-6].

Ir ν_{Os-Br} 226 cm^{-1}.
Homborg, H. *et al, Z. Naturforsch., B*, 1980, **35**, 554 (*synth, ir, uv, raman*)
Schultz, H. *et al, Z. Anorg. Allg. Chem.*, 1983, **502**, 66 (*synth, ir, uv*)

IC-002846

$C_2Br_4S_2$
2,2,4,4-Tetrabromo-1,3-dithietane
Tetrabromo-1,3-dithietane
[62982-84-7]

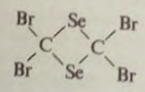


M 407.7
Synth. from corresp. tetrachlorodithietane. Colourless cryst. + BBr_3 (dioxan). Mp 152° dec.
1-Oxide: [97314-82-4].
$C_2Br_4OS_2$ M 423.7
Cryst. (hexane). Mp 91°.
1,1-Dioxide: [73090-25-2].
$C_2Br_4O_2S_2$ M 439.7
Cryst. (CH_2Cl_2/hexane). Mp 135° dec.
1,3-Dioxide: [97314-83-5].
Cryst. (CH_2Cl_2). Mp 159° dec.
1,1,3-Trioxide: [97314-58-4].
$C_2Br_4O_3S_2$ M 455.7
Cryst. (CH_2Cl_2/hexane). Mp 200° dec.
1,1,3,3-Tetroxide: [21511-48-8].
$C_2Br_4O_4S_2$ M 471.7
Cryst. (MeOH). Mp 210° dec.

Opitz, G. *et al, Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 73 (*tetroxide*)
Diderrich, G. *et al, Chem. Ber.*, 1977, **110**, 916 (*synth, ir*)
Seelinger, R. *et al, Angew. Chem., Int. Ed. Engl.*, 1980, **19**, 202 (*tetroxide*)
Rheude, U. *et al, Chem. Ber.*, 1983, **116**, 1285 (*tetroxide*)
Schork, R. *et al, Chem. Ber.*, 1985, **118**, 1415 (*synth, ir, oxides*)
Sundermeyer, W., *Synthesis*, 1988, 349 (*synth*)

IC-002847

$C_2Br_4Se_2$
2,2,4,4-Tetrabromo-1,3-diselenetane

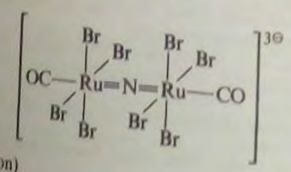


M 501.5
Formed from $F_2C{=}Se$ + BBr_3. Solid, dec. >140° to CSe_2 + CBr_4. Sol. C_6H_6.

Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1976, **427**, 114 (*synth, ir, nu*)

IC-002848

$C_2Br_8NO_2Ru_2^{3\ominus}$
Octabromodicarbonyl-μ-nitridodiruthenate(*IV*)(3−)
μ-Nitridobis[(carbonyl)tetrabromoruthenate(IV)]
[42735-82-0]



M 911.3 (ion)

Sol. aq. HBr.
Tri-Cs salt: Prepd. by treating $[Ru_2NBr_8(OH_2)_2]^{3\ominus}$ in conc. HBr with CO. Yellow-brown salt; diamagnetic. Ir ν_{CO} 2022 cm^{-1}.
Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)

IC-002849

C_2Ca
Calcium carbide (CaC_2), 8CI
Calcium acetylide
[75-20-7]

M 64.1 CaC_2
Structural prototype. Obt. by direct reaction of Ca metal (or CaO) with carbon in an electric furnace; or by reaction of CaH_2 or Ca_3N_2 with carbon. Thermal dec. of calcium cyanamide alone or with carbon in high vacuum also affords CaC_2. Used for production of acetylene by reaction with H_2O. Agent for the desulfurisation of cast iron. Component of fluxes for the dephosphorisation and desulfurisation of stainless steels. Commercially available (80%). Moisture-sensitive. Mp 2300° (extrap). ΔH_f° −60 kJ mol^{-1}; ΔG_f° −65 kJ mol^{-1}; S° 70 J K^{-1} mol^{-1}. Undergoes tetragonal to cubic transition at 450°. Hydrol. in H_2O with formn. of $Ca(OH)_2$ and evolution of C_2H_2. Dissociates to constituent elements at v. high temp. (>2000°).
▷ Flammable; corrosive. EV9400000.

Bredig, M.A., *J. Phys. Chem.*, 1942, **46**, 801 (*polymorphs*)
Atoji, M. *et al, J. Chem. Phys.*, 1959, **31**, 332; 1971, **54**, 3514 (*cryst struct, nd*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 820 (*rev, bibl*)
Bredig, M.A., *Z. Anorg. Allg. Chem.*, 1961, **310**, 338 (*polymorphs*)
Strauss, G. *et al, Ullmanns Encykl. Tech. Chem.*, 4th Ed., 1975, **9**, 70 (*rev, synth, props*)
Strauss, G., *Chemierohst. Kohle*, 1977, **57-66**, 408 (*rev, C_2H_2 prodn*)
Schwob, Y., *Actual. Chim.*, 1978, 32; *CA*, 1979, **90**, 89418 (*rev, synth*)
Haworth, D.T. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 1689 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978, **4**, 432 (*rev*)
Riboud, P. *et al, Circ. Inf. Tech., Cent. Doc. Sider.*, 1979, **36**, 359; *CA*, **91**, 94883 (*rev, desulfurisation*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 665D (*haz*)

IC-002850

C_2CaMgO_6
Calcium magnesium carbonate ($CaMg(CO_3)_2$)
Carbonic acid, calcium magnesium salt (2:1:1), 8CI
[7000-29-5]

$CaMg(CO_3)_2$
M 184.4
Manuf. from the ore by traditional extraction techniques. Prepd. by hydrothermal synth. from either mixtures of $MgCl_2$ and $CaCl_2$ with $(NH_4)_2CO_3$ or mixtures of $MgCO_3$ and $CaCO_3$. Addition of organics such as urea, biuret or ethylenediamine reduces the temp. required for complete reaction. Cement additive for the manuf. of high strength concrete. Also used for the production of fire-resistant building and coating materials. White powder. Dec. on heating with CO_2 loss to form MgO and CaO. Dissolves in acids forming Ca and Mg salts. Prac. insol. H_2O. ΔG_f° −2144 kJ mol^{-1}.
Mineral-form [16389-88-1]
Dolomite

Occurrence widespread. Saddle-shaped cryst., aggregates white, greyish, greenish, pale brown pinkish rhombohedra.

[17069-72-6]

Graf, D.L., *Am. Mineral.*, 1961, **46**, 1283 (*cryst struct*)
Schott, J. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **280**, 1247 (*thermochem data*)
Gilpin, W.C. *et al*, *Proc. Ind. Miner. Int. Congr. 1st*, (1974), 1975, 173 (*rev, uses*)
Langille, D.B. *et al*, *J. Phys. Chem. Solids*, 1977, **38**, 1149 (*ir, raman*)
Brown, A. *et al*, *J. Geol. Educ.*, 1980, **28**, 92 (*rev, ir*)
Otsuka, R. *et al*, *Therm. Anal., Proc. Int. Conf., 6th, 1974*, 1980, **2**, 295 (*thermal dec*)
Maunaye, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Ser. 2*, 1981, **293**, 753 (*synth*)
Mitsushio, H. *et al*, *CA*, 1984, **100**, 44316; **101**, 121843 (*synth*)
Herman, R.G. *et al*, *Mater. Sci. Res.*, 1985, **19**, 113 (*raman*)

C_2CaMnO_6 IC-002851

Calcium manganese(*II*) carbonate ($CaMn(CO_3)_2$)

$CaMn(CO_3)_2$

M 215.0

Occurs in the $CaCO_3/MnCO_3$ system. Prepd. from equimolar mixture of $CaCO_3$ and $MnCO_3$ in a sealed bomb at ~700° and 970 atm. CO_2. Also formed from equimolar amounts of $Mn^{2\oplus}$ and $Ca^{2\oplus}$ in H_2O with excess $(NH_4)_2CO_3$. Synthetic product disordered.

Mineral-form [18616-69-8]
Kutnohorite. *Kutnahorite*
Has ordered struct. related to dolomite. Occurs in USA, Europe (Tuscany, Switzerland, Czechoslovakia), Mexico, Australia, Japan. Pale pink translucent cryst.

Frondel, C. *et al*, *Am. Mineral.*, 1955, **40**, 748 (*struct*)
Goldsmith, J.R. *et al*, *Geochim. Cosmochim. Acta*, 1957, **11**, 310 (*struct, phase studies*)
Graf, D.L., *Am. Mineral.*, 1961, **46**, 1283 (*synth, struct*)
Tsusue, A., *Am. Mineral.*, 1967, **52**, 1751 (*props*)
Clavenna, L.R. *et al*, *CA*, 1978, **88**, 91749 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, *C7*, 222 (*rev, bibl*)

$C_2CaN_2S_2$ IC-002852

Calcium thiocyanate

Thiocyanic acid, calcium salt, 8CI

[2092-16-2]

$Ca(NCS)_2$

M 156.2

Only known as the hydrates or in aq. soln. Attempted synth. in anhyd. solvs. (e.g. reaction of Ca metal with AgNCS in liq. NH_3) gives mixtures of CaS and $Ca(CN)_2$. Aq. solns. synth. by neutralisation of $CaCO_3$ with aq. soln. of HNCS or $[NH_4]NCS$. Cryst. as the tetrahydrate. Attempted dehyd. results in thermal dec. Aq. solns. containing $Ca(NCS)_2$ act as cement setting accelerators. Also used to solubilise cellulose in aq. soln. V. sol. H_2O; sol. MeOH, EtOH.

▷ XK8540000.

Trihydrate: [5892-22-8].
$C_2H_6CaN_2O_3S_2$ M 210.2
Obt. by dehyd. of the tetrahydrate over conc. H_2SO_4 or *in vacuo* over P_2O_5. Deliquescent white cryst. V. sol. H_2O, EtOH.

Tetrahydrate: [65114-14-9].
$C_2H_8CaN_2O_4S_2$ M 228.3
Cryst. from aq. solns. of CaSCN. V. sol. H_2O (150 g per 100 cm^3 at 25°; 173 g per 100 cm^3 at 50°).

Burgess, W.M. *et al*, *J. Am. Chem. Soc.*, 1937, **59**, 462 (*anhyd attempted synth*)
Tramer, A., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1961, **253**, 1786 (*ir, raman, tetrahydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 972, 973 (*rev, bibl*)
Sare, J. *et al*, *J. Phys. Chem.*, 1973, **77**, 1869 (*pmr*;7Kargol, J.A. *et al*, *Inorg. Chem.*, 1979, **18**, 2532 (*cmr*)
Kuga, S., *J. Colloid Interface Sci.*, 1980, **77**, 413 (*use*)
Perelygin, I.S. *et al*, *Zh. Strukt. Khim.*, 1983, **24**, 67 (*ir*)
Baranovskii, V.I. *et al*, *Khim. Fiz.*, 1985, **4**, 528 (*Na-23, H-2 nmr*)
Japan. Pat., 61 155 236, (1986); *CA*, **105**, 231509 (*use*)

C_2CaO_4 IC-002853

Calcium oxalate

Calcium ethanedioate. Ethanedioic acid, calcium salt, 9CI. Oxalic acid, calcium salt, 8CI

[563-72-4]

$Ca(C_2O_4)$

M 128.0

Exists in 3 modifications which interconvert at 250-370° ($\alpha \rightarrow \beta$) and 410° ($\beta \rightarrow \gamma$). Prepd. either by thermal dec. of calcium formate at 400° or by dehyd. of its hydrates at 200-300°. Commercially available as hydrate. The hydrates are of considerable medical interest since they occur in renal and urinary calculi. White powder. Dec. on heating with CO and CO_2 loss forming $CaCO_3$ at 410-475° and CaO at 860°. Dissolves in acids. Prac. insol. H_2O (6.7×10^{-4} g per 100 cm^3 at 13°; 1.4×10^{-3} g per 100 cm^3 at 95°); insol. AcOH. ΔH_f° −1361 kJ mol^{-1}.

Monohydrate: [14488-96-1]. ***Whewellite***
$C_2H_2CaO_5$ M 146.1
Prep. by reaction of $CaCl_2$ with aq. $H_2C_2O_4$. Also found as mineral in Germany, Italy, USSR and elsewhere. Formed in human urine and found in renal and urinary calculi and as an intracellular deposit in plants. Colourless monoclinic cryst. Dec. on heating with H_2O loss at 235° to form anhyd. calcium oxalate. Prac. insol. H_2O. ΔH_f° −1675 kJ mol^{-1}; ΔG_f° −1514 kJ mol^{-1}; S° 157 J K^{-1} mol^{-1}.

Dihydrate: [7236-42-2]. ***Weddellite***
$C_2H_4CaO_6$ M 164.1
Found as mineral in oceanic bottom sample from Antarctica. Also formed in human urine and found in renal and urinary calculi. Capable of absorbing up to $\frac{1}{2}$ mole of zeolitic water. Colourless tetragonal cryst.; mineral, tan, yellowish brown to brown due to org. impurities. Dec. on heating with H_2O loss at 120° to form whewellite and with CO and CO_2 loss to form $CaCO_3$ and CaO. Prac. insol. H_2O. ΔH_f° −1968 kJ mol^{-1}; ΔG_f° −1750 kJ mol^{-1}.

Rossini, F.D. *et al*, *Natl. Bur. Std. Circ. (U.S.)*, No. 500, 1952, 395 (*thermochem data, hydrates*)
von Philipsborn, H., *Protoplasmatologia*, 1952, **41**, 415 (*dihydrate, zeolitic water abs*)
Hoffmann, W., *Naturwissenschaften*, 1960, **47**, 38 (*cryst struct, monohydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 996, 1000, 1001 (*rev, bibl, hydrates, anhyd*)
Walter-Levy, L. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1962, **254**, 296; 1964, **259**, 4685 (*hydrates, cryst from soln, synth, hydrates, anhyd, thermal dec*)
Sterling, C., *Science (Washington, D.C.)*, 1964, **146**, 158 (*dihydrate, formn renal calculi*)
Hocart, R. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **260**, 2509 (*polymorphs*)

Hutton, C.O. *et al*, *Mineral. Mag.*, 1965, **34**, 256 (*dihydrate, cryst struct*)
Arnott, H.J. *et al*, *Nature (London)*, 1965, **208**, 1197 (*formn in plants, monohydrate*)
Gerard, N. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1966, **261**, 2363 (*polymorphs*)
Shippey, T.A., *J. Mol. Struct.*, 1980, **63**, 157 (*ir, raman, anhyd, monohydrate*)
Schubert, G. *et al*, *Cryst. Res. Technol.*, 1981, **16**, 1025 (*polymorphs, monohydrate*)
Young, R.A. *et al*, *Life Sci. Res. Rep.*, (Biol. Miner. Deminer.), 1982, **23**, 101; *CA*, **97**, 34773 (*struct*)
Duval, D. *et al*, *Phys. Status Solidi B*, 1985, **132**, 83 (*raman, monohydrate*)

$C_2Ca_5O_{13}Si_2$ IC-002854

Tilleyite

Calcium carbonate pyrosilicate ($Ca_5(CO_3)_2(Si_2O_7)$)

[12261-87-9]

$Ca_5[Si_2O_7][CO_3]_2$

M 488.5

Mineral. Colourless or white cryst.

Louisnathan, S.J. *et al*, *Z. Kristallogr.*, 1970, **132**, 288 (*cryst struct*)
Henmi, C. *et al*, *Mineral. J.*, 1978, **9**, 106 (*synth*)

$C_2CdF_6Te_2$ IC-002855

Bis(trifluoromethanetellurolato)cadmium

Cadmium trifluoromethyltelluride. Trifluoromethanetellurol, cadmium salt

[111051-78-6]

$F_3CTeCdTeCF_3$

M 505.6

Synth. from Cd + $(F_3C)_2Te_2$ in DMF at 20°. Brown oil; dec. in light.

Kischkewitz, J. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **547**, 167 (*synth, F-19 nmr*)

C_2CdN_2 IC-002856

Cadmium cyanide ($Cd(CN)_2$)

[542-83-6]

$Cd(CN)_2$

M 164.4

Cu_2O-type struct. Synth. from $Cd(OH)_2$ and HCN, or from $Cd(OAc)_2$ in EtOH and HCN in Et_2O. Air-stable white cryst.; turns brown on heating in air. Sol. H_2O (1.7 g per 100 cm^3 at 15°), strong acids, excess $CN^{\ominus}$; sl. sol. EtOH. Dec. > 200°.

Blitz, W., *Z. Anorg. Allg. Chem.*, 1928, **170**, 161.
Shugam, E. *et al*, *Acta Physicochim., USSR*, 1945, **20**, 247 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 33, 1959, 656.
Swanson, H.E. *et al*, *NBS Monogr. (U.S.)*, *No.* 25, 1963 (*powder struct*)
Wyckoff, R.W.G., *Crystal Structures*, Interscience, N.Y., 1965, **3**, 580.
Haas, H. *et al*, *J. Chem. Phys.*, 1973, **58**, 3339 (*nqr*)
Dehnicke, G. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1974, **78**, 1010 (*ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1050 (*synth*)
Abrahams, B.F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1990, 60 (*honeycomb form, cryst struct, solvate*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 667 (*tox*)

$C_2CdN_2S_2$ IC-002857

Cadmium thiocyanate

Bis(thiocyanato)cadmium. Thiocyanic acid, cadmium salt

[865-38-3]

$Cd(NCS)_2$

M 228.5

Solid state contains 6-coord. octahedral Cd (4 S + 2 *trans* N); bridging NCS provide 8-membered rings. Reported to be Cd—S coord. in DMSO and Cd—N coord. in H_2O. Synth. from $CdSO_4$ and $Ba(SCN)_2$ in H_2O. Colourless cryst. (H_2O or EtOH). K_{sp} 2.51×10^{-5}.

Spacu, G. *et al*, *Z. Anorg. Allg. Chem.*, 1936, **227**, 385 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 33, 1959, 658.
Ferraro, J.R. *et al*, *Spectrochim. Acta*, 1961, **17**, 802 (*raman, solid*)
Flint, C.D. *et al*, *J. Chem. Soc. A*, 1970, 442 (*synth, ir*)
Cardin, A.D. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 1672 (*Cd-113 nmr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1051 (*synth*)
Cannas, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 300 (*cryst struct, synth*)
Zurano Hernandez, G. *et al*, *An. Quim.*, 1977, **73**, 820 (*cryst struct*)
Persson, I. *et al*, *Acta Chem. Scand., Ser. A*, 1981, **35**, 295 (*soln raman*)
Goel, R.G., *Spectrochim. Acta, Part A*, 1981, **37**, 557 (*ir, raman*)
Böhland, H. *et al*, *Z. Chem.*, 1986, **26**, 184 (*pe*)

C_2CdO_4

Cadmium oxalate

[814-88-0]

$Cd(C_2O_4)$

M 200.4

Amorphous powder. Mp 340° dec.

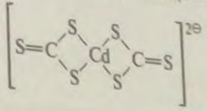
Trihydrate: [20712-42-9].
$C_2H_6CdO_7$ M 254.4
Prepd. from Cd salts + oxalic acid. White needles.

Gmelin Handbook Inorg. Chem., Syst. No. 33, *Suppl. Vol*, 1959, 653 (*rev*)
Bridle, C. *et al*, *Acta Crystallogr.*, 1965, **19**, 483 (*cryst struct, trihydrate*)

$C_2CdS_6^{2\ominus}$ IC-002859

Bis(trithiocarbonato)cadmate(2−)

Bis[carbonotrithioato(2−)-S,S']cadmate(2−), 9CI



M 328.8 (ion)

Formed from $CdCl_2$ + $[CS_3]^{2\ominus}$.

Bis-Ph_4P salt: [51436-00-1].
Light yellow cryst.

Bis-Ph_4As salt: [51436-01-2].
Light yellow cryst.

Mueller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **401**, 274 (*synth, uv, ir*)

$C_2ClCoNO_3^{\ominus}$ IC-002860

Dicarbonylchloronitrosylcobaltate(1−), 8CI

$[CoCl(CO)_2NO]^{\ominus}$

M 180.4 (ion)

Reacts with benzyl halides to give benzaldoxime, PhCH=NOH.

Tetraheptylammonium salt: [33393-84-9].
Ir ν_{CO} 2012, 1938, ν_{SO} 1703 cm^{-1} (diglyme).

Foa, M. *et al*, *J. Organomet. Chem.*, 1971, **30**, 123 (*synth, ir*)

IC-002861

C_2ClF_2NSe

Chlorodifluoromethyl selenocyanate

Selenocyanic acid chlorodifluoromethyl ester

[54451-31-9]

$F_2ClCSeCN$

M 190.4
Formed from $F_2ClCSeCl$ + AgCN at 20°. Colourless liq. Bp 112°.

Haas, A. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **427**, 114 (*synth, ir, ms, F-19 nmr*)

IC-002862

C_2ClF_3

Chlorotrifluoroethylene

Chlorotrifluoroethene, 9Cl. CTFE. Fluorocarbon 1113. Kel F

[79-38-9]

$ClFC{=}CF_2$

M 116.4
Refrigerant and monomer for production of polymers. Gas. d_4^0 1.38. Fp −157.5° (−157.9°). Bp −26.2° (−27.9°).

▷ Toxic, extremely flammable. Violent reacn. with some substances. KV0525000.

U.K. Pat., 698 386, (1955); *CA*, **49**, 3237.
U.S. Pat., 2 667 518, (1955); *CA*, **49**, 2478.
Yakubovich, A.Ya. *et al*, *CA*, 1956, **50**, 206.
Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 94.
Blancou, H. *et al*, *J. Fluorine Chem.*, 1977, **9**, 309 (*synth*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 336.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 898.

IC-002863

C_2ClF_5

Chloropentafluoroethane

Fluorocarbon 115. Freon 115. Arcton 115

[76-15-3]

F_5CCClF_2

M 154.4
Manuf. by reaction of tetrachloroethene with Cl_2 and HF over Cr_2O_3 catalysts. Low-temp. refrigerant component. Gas. Mp −106°. Bp −37.7°.

▷ Low toxicity, OES 6320 mg m^{-3}. Non-flammable. Substance production controlled by environmental legislation. KH7877500.

Haszeldine, R.N., *J. Chem. Soc.*, 1953, 3761.
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 860.

IC-002864

$C_2ClF_6NO_4S_2$

N-Chlorobis(trifluoromethylsulfonyl)imide

N-Chloro-1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl] methanesulfonamide, 9Cl. N-Chloroimidobis(trifluoromethyldisulfuryl) fluoride

[91742-17-5]

$ClN(SO_2CF_3)_2$

M 315.6
From Bis[(trifluoromethyl)sulfonyl]imide, IC-002989 + ClF in $CFCl_3$ at 0°. Volatile viscous liq. with acrid smell; glass at −196°. Mp −96° to −93°. V.p. 8 mm at 22°.

▷ Explosive.

Foropoulos, J.J. *et al*, *Inorg. Chem.*, 1984, **23**, 3720 (*synth, ir, raman, ms, F-19 nmr*)

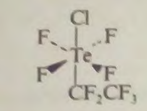
IC-002865

C_2ClF_9Te

Chlorotetrafluoro(pentafluoroethyl)tellurium(*VI*)

Perfluoroethyltellurium monochloride tetrafluoride

[51255-74-4]



M 358.0
trans-Octahedral. Gel-like solid or colourless liq. Mp −78°. V.p. ~ 70 mm at r.t.

Lau, C. *et al*, *Can. J. Chem.*, 1985, **63**, 2273 (*ir, synth, raman, F-19 nmr*)

IC-002866

$C_2ClMgNa_3O_6$

Magnesium sodium carbonate chloride ($MgNa_3(CO_3)_2Cl$)

$Na_3Mg(CO_3)_2Cl$

M 248.7
Synth. by reaction of Na_2CO_3 and NaCl in H_2O followed by addition of $MgCl_2.6H_2O$.

Mineral-form [12180-11-9]
Northupite
Colourless to yellowish-grey cubic cryst.

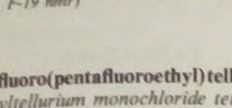
Shiba, H. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1931, **193**, 1421 (*cryst struct*)
Watanabe, T., *Sci. Pap. Inst. Phys. Chem. Res. (Jpn.)*, 1933, **21**, 35; *CA*, 1933, **27**, 4193[1] (*synth*)
Alder, H.H., *Am. Mineral.*, 1963, **48**, 839 (*ir*)
Pemberton, H.E., *Mineral. Rec.*, 1975, **6**, 74 (*rev*)

IC-002867

C_2ClO_2Rh

Dicarbonylchlororhodium

Dicarbonylrhodium chloride



dimer

M 194.3
Dimeric.

Dimer: [14523-22-9]. *Tetracarbonyldi-μ-chlorodirhodium, 9Cl. Bis(chlorodicarbonylrhodium)*
$C_4Cl_2O_4Rh_2$ M 388.7

Catalyst for strained hydrocarbon rearrangements and olefin hydroformylation. Starting material for Rh(I) carbonyl compds. Red needles. Insol. hydrocarbons. Mp 126.5-127°. Solns. dec. slowly in air. Ir ν_{CO} 2115w, 2095s, 2045s cm^{-1} (nujol).

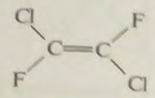
Dahl, L.F. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 1761 (*struct*)
Clement, D.I. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 1509 (*nmr*)
Colton, R. *et al*, *Aust. J. Chem.*, 1970, **23**, 1351 (*synth, ir*)
Gallay, J. *et al*, *J. Organomet. Chem.*, 1972, **38**, 179 (*synth, ir*)
Inorg. Synth., 1974, **15**, 14, 17 (*synth*)
Sakakibara, T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 458 (*use*)
Iqbal, M.Z., *CA*, 1980, **93**, 87637 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1982, **10**, 382.

IC-002868

$C_2Cl_2F_2$

1,2-Dichloro-1,2-difluoroethene

Fluorocarbon 1112



M 132.9
(E)-form [381-71-5]
d_4^0 1.494. Mp −93.3°, Fp −110.3°. Bp 22°.

[598-88-9, 27156-03-2]

Mann, D.E. *et al*, *J. Chem. Phys.*, 1957, **26**, 773 (*ir, raman*)
Stacey, M. *et al*, *Adv. Fluorine Chem.*, Butterworths, London, 1963, **3**, 175.
Craig, N.C. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 4223 (*synth, ir, raman*)
Synatka, B.G. *et al*, *Zh. Org. Khim.*, 1972, **8**, 1553 (*ms*)
Takada, K. *et al*, *Org. Magn. Reson.*, 1977, **9**, 116 (*F-19 nmr*)

IC-002869

$C_2Cl_2F_2$

1,1-Dichloro-2,2-difluoroethylene, 8Cl

1,1-Dichloro-2,2-difluoroethene, 9Cl. Fluorocarbon 1112a

[79-35-6]

$F_2C{=}CCl_2$

M 132.9
Volatile liq. Fp −127.1° to −126.7 (−115°). $Bp_{764.3}$ 20.4°.

▷ Toxic. Emits highly toxic fumes when heated to dec.. KV9470000.

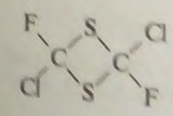
Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)
Org. Synth., Coll. Vol., **4**, 1963, 268 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 117.
Abraham, R.J. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1973, 1027 (*nmr*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1142.

IC-002870

$C_2Cl_2F_2S_2$

2,4-Dichloro-2,4-difluoro-1,3-dithietane

[62982-86-9]



M 197.0
Mixt. of *cis* and *trans* isomers. Synth. from Thiocarbonyl chloride fluoride, IC-002327 and SbF_5/HF. Colourless liq. Bp_{53} 56°.

IC-002871

$C_2Cl_2F_4$

1,1-Dichloro-1,2,2,2-tetrafluoroethane

Fluorocarbon 114a

[374-07-2]

F_3CCFCl_2

M 170.9
Refrigerant component. d_4^{25} 1.455. Fp −56.6°. Bp 3.0°. n_D^0 1.3092.

▷ Irritant.

[1320-37-2]

Nielsen, J.R. *et al*, *J. Chem. Phys.*, 1953, **21**, 383 (*ir, raman*)
Goldwhite, H. *et al*, *J. Chem. Soc.*, 1961, 3825 (*synth, ir*)
Vecchio, M. *et al*, *J. Fluorine Chem.*, 1974, **4**, 117 (*synth*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Eujen, R. *et al*, *J. Fluorine Chem.*, 1983, **22**, 263 (*F-19 nmr*)

IC-002872

$C_2Cl_2F_4$

1,2-Dichloro-1,1,2,2-tetrafluoroethane, 9Cl, 8Cl

Fluorocarbon 114. Arcton 114. Freon 114

[76-14-2]

$ClCF_2CF_2Cl$

M 170.9
Manuf. by the reaction of tetrachloroethene with HF and chlorine over Cr_2O_3 catalyst. Important aerosol propellant. Refrigerant. Anaesthetic. Gas. d_4^0 1.531. Mp −94°. Bp 3.8°. n_D^{25} 1.3092.

▷ Narcotic at high concs., OES (TLV) 7000 mg m^{-3}. Reacts violentlywith Al. Production controlled by environmental legislation. KI1101000.

Locke, E.G. *et al*, *J. Am. Chem. Soc.*, 1934, **56**, 1726 (*synth*)
Harris, R.K. *et al*, *Trans. Faraday Soc.*, 1963, **59**, 806 (*nmr*)
Brown, F.B. *et al*, *J. Mol. Spectrosc.*, 1967, **24**, 163 (*ir, raman*)
Doucet, J. *et al*, *J. Chem. Phys.*, 1975, **62**, 355 (*ac*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1775.

1-Oxide: [108319-75-1].
$C_2Cl_2F_4OS_2$ M 213.0
Colourless liq. Bp_{15} 62-70°. Three stereoisomers identified.
1,1-Dioxide: [108319-77-3].
$C_2Cl_2F_4O_2S_2$ M 229.0
Colourless liq. Sol. CH_2Cl_2. Bp_3 43°.
1,3-Dioxide: [108391-95-3].
White cryst. Sol. CH_2Cl_2. Mp 105-106°.
1,1,3-Trioxide: [108319-76-2].
$C_2Cl_2F_4O_3S_2$ M 245.0
Colourless liq. Sol. CH_2Cl_2, sl. sol. pet. ether. $Bp_{1.3}$ 85-87°. Formed as mixt. of 3 stereoisomers.
1,1,3,3-Tetraoxide: [108319-78-4].
$C_2Cl_2F_4O_4S_2$ M 261.0
Colourless cryst. (by subl.). Mp 120-127°. Formed as mixt. of 2 isomers.
[62982-87-0, 108319-89-7, 108391-96-4, 108391-97-5, 108391-98-6, 108448-26-6]

Diderrich, G. *et al*, *Chem. Ber.*, 1977, **110**, 916 (*synth, ir, F-19 nmr*)
Haas, A. *et al*, *Chem. Ber.*, 1987, **120**, 429 (*synth, reactions*)
Henn, R. *et al*, *Chem. Ber.*, 1987, **120**, 1499 (*deriv, synth, ir, ms, F-19 nmr*)

IC-002873

$C_2Cl_2F_4Se$

Bis(chlorodifluoromethyl) diselenide, 9CI

1,3-Dichloro-1,1,3,3-tetrafluoro-2-selenapropane. Bis(chlorodifluoromethyl)selane

[54393-43-0]

$F_2ClCSeCClF_2$

M 249.8

Formed from $F_2C{=}Se + Cl_2$ at −60°. Red liq. Bp 77-78°.

Haas, A. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **427**, 114 (*synth, ir, ms, F-19 nmr*)

IC-002874

$C_2Cl_2IrO_2^{\ominus}$

Dicarbonyldichloroiridate(1−), 10CI

As Dibromodicarbonyliridate(1−), IC-002834 with

X = Cl

M 319.1 (ion)

cis-form

Ph_4As salt: [15152-88-2]

Yellow cryst. Ir ν_{CO} 2056, 1975 cm^{-1} ($MeNO_2$).

Bonati, F. *et al*, *J. Organomet. Chem.*, 1967, **7**, 167 (*synth*)
Forster, D. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 433 (*synth, ir*)
Forster, D., *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 221 (*synth, ir*)
Piraino, P. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 1237 (*synth, ir*)

IC-002875

$C_2Cl_2IrO_2$

Dicarbonyldichloroiridium

$[Ir(CO)_2Cl_2]_n$

M 319.1

Polymeric, *n* unknown. Lustrous white needles. Mp 140° dec. Subl. 150° in a stream of CO. Rapidly dec. by water but stable in dry air.

Manchot, W. *et al*, *Ber.*, 1925, **58**, 232 (*synth*)
Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1941, **246**, 138 (*synth*)

IC-002876

$C_2Cl_2O_2Pd$

Dicarbonyldichloropalladium, 9CI

Dicarbonylpalladium dichloride

[13682-72-9]

$PdCl_2(CO)_2$

M 233.3

Prepd. from CO and $PdCl_2(NCPh)_2$. Catalyses conversion of aromatic nitro compds. by CO to isocyanates. No phys. details available.

Yamahara, T. *et al*, *CA*, 1974, **80**, 120518y (*synth, use*)

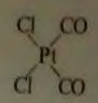
IC-002877

$C_2Cl_2O_2Pt$

Dicarbonyldichloroplatinum, 10CI

Dichloroplatinum dicarbonyl. Dicarbonylplatinum chloride

[25478-60-8]



cis-form

M 322.0

Hydroformylation catalyst.

cis-form [15020-32-3]

More stable form. Cryst., stored in sealed tube under refrigeration. Subl. 200°. Ir ν_{CO} 2179, 2136 cm^{-1}.

trans-form [62841-60-5]

Less stable form. Cryst. ($SOCl_2$/hexane). Ir ν_{CO} 2150 cm^{-1}. Stable at −78°. Dec. at r.t. to *cis*-form and $[Pt_2Cl_4(CO)_2]$. Unstable to light.

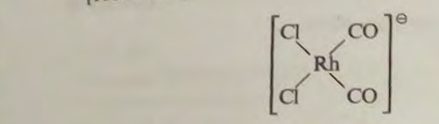
Saito, Y. *et al*, *Seisan Kenkyu*, 1976, **28**, 440; *CA*, **86**, 170267k (*synth, ir, nmr*)
Dell'Amico, D.B. *et al*, *Gazz. Chim. Ital.*, 1977, **107**, 101 (*synth*)
Browning, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, raman, nmr*)
Dell'Amico, D.B. *et al*, *Inorg. Chem.*, 1984, **23**, 3030, 4781 (*synth, ir, Pt-195 nmr*)
Andreini, B.P. *et al*, *J. Organomet. Chem.*, 1988, **354**, 357 (*ir, cmr, props*)

IC-002878

$C_2Cl_2O_2Rh^{\ominus}$

Dicarbonyldichlororhodate(1−), 10CI

[15550-00-2]



M 229.8 (ion)

Starting material for CO-containing Rh complexes. Catalyst for the reduction of NO by CO.

cis-form [44516-52-1]

Tetrabutylammonium salt: [17966-76-6].

Pale-yellow cryst. (C_6H_6/hexane). Mp 81° dec. Ir ν_{CO} 2060, 1975 cm^{-1} (nujol).

Ph_4As salt: [30193-19-2].

Pale-yellow cryst. (Me_2CO/pet. ether). Mp 185-190°, Mp 181° dec. Ir ν_{CO} 2058, 1974 cm^{-1} (nujol).

Vallarino, L.M., *Inorg. Chem.*, 1965, **4**, 161 (*synth, ir*)
Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1970, 2788 (*synth, ir*)
Stanko, J.A. *et al*, *Inorg. Chem.*, 1971, **10**, 566 (*synth, struct*)
Varshavskii, Yu.S. *et al*, *J. Organomet. Chem.*, 1971, **31**, 119 (*use*)
Meyer, C.D. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1364 (*use*)
Hendrikson, D.E. *et al*, *Inorg. Chem.*, 1977, **16**, 970 (*use*)
Brown, C. *et al*, *J. Organomet. Chem.*, 1980, **192**, 93 (*nmr*)

IC-002879

$C_2Cl_2O_2Ru$

Dicarbonyldichlororuthenium, 9CI

$Ru(CO)_2Cl_2$

M 227.9

Monomeric and polymeric forms known.

Monomer: [16369-40-7].

Fine yellow cryst.

Colton, R. *et al*, *Aust. J. Chem.*, 1967, **20**, 1283 (*synth, ir*)
Cleare, M.J., *Platinum Met. Rev.*, 1967, **11**, 148 (*synth*)
Berch, M.L. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 3763 (*synth*)

IC-002880

C_2Cl_3F

Trichlorofluoroethylene, 8CI

Trichlorofluoroethene, 9CI. Fluorocarbon 1111

[359-29-5]

$Cl_2C{=}CClF$

M 149.3

d_4^{20} 1.55. Mp −108.9°. Bp 71°.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 1025 (*props*)
Italian Pat., 804 231, (1968); *CA*, **71**, 60667 (*synth*)

IC-002881

$C_2Cl_3F_3$

1,1,1-Trichloro-2,2,2-trifluoroethane, 8CI

Fluorocarbon 113a

[354-58-5]

F_3CCCl_3

M 187.3

Prepd. by isom. of CCl_2FCClF_2 using $AlCl_3$ catalyst. Blowing agent, propellant, refrigerant, synthetic intermed. Liq. d_4^{20} 1.58. Fp 14°. Bp 46°.

Miller, W.T. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 705.
Hamilton, J.M., *Adv. Fluorine Chem.*, 1963, **3**, 117 (*rev*)
Banks, R.E., *Organofluorine Chem. their Ind. Appl.* [*Symp.*], Soc. of Chem. Ind., London, 1979, 62, 79 (*rev, use, manuf*)

IC-002882

$C_2Cl_3F_3$

1,1,2-Trichloro-1,2,2-trifluoroethane

Fluorocarbon 113. Freon 113. Arcton 113. Arklone P. Genetron 113

[76-13-1]

$Cl_2CFCClF_2$

M 187.3

Manuf. from reaction of tetrachloroethene and anhydrous HF using antimony chlorofluoride catalyst. Solvent (esp. for degreasing of electrical components), polymer intermed., blowing agent, intermed. for org. synth. Mp −36.4°. Bp 47.7°.

▷ Reacts violently with some metals. Low toxicity, OES 1000 ppmv/v. Production controlled by environmental legislation. KJ4000000.

Iwasaki, M., *Bull. Chem. Soc. Jpn.*, 1959, **32**, 194 (*struct*)
Case, J.R. *et al*, *J. Chem. Soc.*, 1961, 2070 (*synth*)
Park, J.D. *et al*, *J. Org. Chem.*, 1961, **26**, 3316, 3319, 4017 (*synth*)
Vecchio, M., *Hydrocarbon Process.*, 1973, **52**, 97 (*synth*)
Naae, D.G. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Kolditz, L. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **434**, 55 (*synth*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 517.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1775.

IC-002883

$C_2Cl_3NO_5Ru^{2\ominus}$

Trichloro(nitrosyl)(oxalato)ruthenate(2−)

Trichloro(ethanedioato-O,O′)(nitrosyl)ruthenate(2−)

$[Ru(NO)Cl_3(C_2O_4)]^{2\ominus}$

M 325.4 (ion)

Isomeric form unknown.

Di-K salt:

$C_2Cl_3K_2NO_5Ru$ M 403.6

No phys. props. reported.

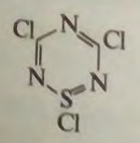
Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 188 (*synth*)

IC-002884

$C_2Cl_3N_3S$

1,3,5-Trichloro-1*H*-1,2,4,6-thiatriazine, 9CI

[58589-34-7]



M 204.4

Synth. from $SOCl_2$ + $NaN(CN)_2$. White cryst. or yellow oil, readily hydrol. Mp 32-34°. Bp_2 70°.

Geevers, J., *J. Chem. Soc. C*, 1970, 875 (*synth*)
Voss, G. *et al*, *Z. Chem.*, 1976, **16**, 358 (*synth, struct, cmr, ms*)

IC-002885

$C_2Cl_3NaO_2$

Sodium trichloroacetate

Trichloroacetic acid, sodium salt, 8CI. 2,2,2-Trichloroethanoic acid, sodium salt

[650-51-1]

$NaOOCCCl_3$

M 185.3

Synth. by neutralisation of Na_2CO_3 by aq. CCl_3COOH. Manuf. by two stage chlorination of Me_2CO followed by digestion with aq. NaOH. Commercially available. Herbicide. Component of some thermal recording papers. White powder. Sol. H_2O. Mp > 300°.

▷ Irritant. AJ9100000.

Leopold, A.C., *Weeds*, 1960, **8**, 48; *CA*, **54**, 21608b (*soly*)
Ambrus, T. *et al*, *Rev. Chim. (Bucharest)*, 1963, **14**, 506; *CA*, 1964, **60**, 6739f (*manuf*)
Spinner, E., *J. Chem. Soc.*, 1964, 4217 (*ir, raman*)
Hartman, K.A., *J. Chem. Phys.*, 1966, **70**, 270 (*pmr*)
Kanekar, C.R. *et al*, *Proc. Chem. Symp., 1st*, 1969, **2**, 265; *CA*, 1971, **74**, 69746 (*ir*)
Hashimoto, M., *Chem. Lett.*, 1975, 1325 (*Cl-35 nqr*)
Evsikov, V.D., *CA*, 1984, **101**, 105719 (*use, herbicide*)
Japan. Pat., 59 150 792, (1984); *CA*, 1985, **102**, 140978 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3402D (*haz*)

C_2Cl_4

Tetrachloroethylene, USAN

IC-002886

Tetrachloroethene, 9CI. Perchloroethylene. Perclene. Perklone. Nema. Ankilostin. Didakene. Kosmocermil. Tetracap. Tetropil. Verminol

[127-18-4]

$Cl_2C{=}CCl_2$

M 165.8

Manuf. by pyrolysis of CCl_4. Widely used non-flammable solv. Used in drycleaning, degreasing and textile finishing. Anthelmintic, effective against hookworms and intestinal flukes. Used in manuf. of fluorocarbons. Liq. with ether-like odour. d_4^{20} 1.62. Fp −22.35°, Mp −19°. Bp 121°, Bp_{30} 33.2°.

▷ Mod. toxic, OES 335 mg m^{-3}. KX3850000.

Weisen, H.B. *et al*, *J. Phys. Chem.*, 1919, **23**, 415.
Timmermans, J. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1930, **27**, 401.
U.S. Pat., 1 947 491, (1934); *CA*, **28**, 2371 (*synth*)
Frydlender, J.H., *CA*, 1935, **29**, 7935 (*rev*)
Hawkes, G.E. *et al*, *J. Org. Chem.*, 1974, **39**, 1276 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 754 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 813.
Reichert, D., *Mutat. Res.*, 1983, **123**, 411 (*metab, inv*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 497.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3190.

$C_2Cl_4F_2$ IC-002887

1,1,2,2-Tetrachloro-1,2-difluoroethane

Fluorocarbon 112. 1,2-Difluoro-1,1,2,2-tetrachloroethane

[76-12-0]

$Cl_2CFCFCl_2$

M 203.8

Degreasing solvent. Cryst. Mp 24.65°. Bp 92.8°.

▷ OES 834 mg m^{-3}. Production controlled by environmental legislation. KI1420000.

Locke, E.G. *et al, J. Am. Chem. Soc.*, 1934, **56**, 1726 (*synth*)
Miller, W.T. *et al, J. Am. Chem. Soc.*, 1937, **59**, 198 (*synth*)
Kakac, B. *et al, Collect. Czech. Chem. Commun.*, 1965, **30**, 745 (*ir*)
Newmark, R. *et al, J. Phys. Chem.*, 1968, **72**, 4299 (*nmr*)
Hawkes, G.E. *et al, J. Org. Chem.*, 1974, **39**, 1276 (*cmr*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 497.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1255.

$C_2Cl_4IrO_2^{\ominus}$ IC-002888

Dicarbonyltetrachloroiridate(1−)

As Tetrabromodicarbonyliridate(1−), IC-002840 with

X = Cl

M 390.0 (ion)

cis-form

K salt: [53728-62-4].
No phys. props. reported.

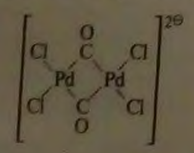
Ph_4As salt: [36487-39-5].
Pale-yellow cryst. Ir ν_{CO} 2143, 2094 cm^{-1} ($MeNO_2$).

Forster, D., *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 221 (*synth, ir*)
Forster, D., *Inorg. Chem.*, 1972, **11**, 433 (*synth*)

$C_2Cl_4O_2Pd_2^{2\ominus}$ IC-002889

Dicarbonyltetrachlorodipalladate(2−), 10Cl

Dicarbonyldi-μ-chlorodichlorodipalladate(2−), 9Cl (incorr.)



M 410.6 (ion)

Contrary to 9Cl name, believed to have CO bridges.

Synth. from Tetrachloropalladate(*II*)(2−), IC-017115 + CO. One of many Pd complexes catalysing $PhNO_2$ + CO → PhNCO + CO_2.

Di-Cs salt: [51233-15-9].
Pale yellow solid.

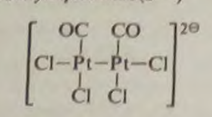
Bis-tetrabutylammonium salt: [78833-56-4].
Waxy yellow solid. Sol. CH_2Cl_2.

Colton, R. *et al, Aust. J. Chem.*, 1973, **26**, 2607 (*synth, ir*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 534 (*synth, ir, raman*)
Tietz, H. *et al, Z. Chem.*, 1980, **20**, 256, 295, 411 (*use*)

$C_2Cl_4O_2Pt_2^{2\ominus}$ IC-002890

Dicarbonyltetrachlorodiplatinate(2−), 9Cl

Tetrachlorodicarbonyldiplatinate(2−)



M 587.9 (ion)

Bis(tetrapropylammonium) salt: [52538-93-9].
$C_{26}H_{56}Cl_4N_2O_2Pt_2$ M 960.7
Yellow solid (Et_2O). Mp 188° dec.

Bis(tetrabutylammonium) salt: [83789-27-9].
$C_{34}H_{72}Cl_4N_2O_2Pt_2$ M 1072.9
Yellow-green cryst. (tripropylamine/formic acid). Mp 165°.

Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2355 (*synth, ir*)
Modinos, A. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1516 (*struct*)
Boag, N.M. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1101 (*synth, nmr*)

$C_2Cl_4O_2Rh^{\ominus}$ IC-002891

Dicarbonyltetrachlororhodate(1−)

Tetrachlorodicarbonylrhodate(1−)

$[RhCl_4(CO)_2]^{\ominus}$

M 300.7 (ion)

Characterised spectroscopically.

cis-form

Ir ν_{CO} 2160s, 2125s cm^{-1} ($CHCl_3$).

Forster, D., *Inorg. Chem.*, 1969, **8**, 2556 (*synth, ir*)

$C_2Cl_4O_2Ru^{2\ominus}$ IC-002892

Dicarbonyltetrachlororuthenate(2−), 9Cl, 8Cl

[60105-91-1]

$[RuCl_4(CO)_2]^{2\ominus}$

M 298.9 (ion)

cis-form

Di-Cs salt: [17439-05-3].
$C_2Cl_4Cs_2O_2Ru$ M 564.7
Bright-yellow cryst.

Bis-Ph_4As salt: [51982-86-6].
Yellow cryst. (CH_2Cl_2/pet. ether).

Halpern, J. *et al, J. Am. Chem. Soc.*, 1966, **88**, 5142 (*synth, spectra*)
Cleare, M.J. *et al, J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Colton, R. *et al, Aust. J. Chem.*, 1971, **24**, 903 (*synth, ir*)
Stephenson, T.A. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2112 (*synth*)

$C_2Cl_4O_4Os^{2\ominus}$ IC-002893

Tetrachloro(oxalato)osmate(*IV*)(2−)

[74325-52-3]

As Tetrabromo(oxalato)osmate(*IV*)(2−), IC-002845 with

X = Cl

M 420.0 (ion)

Synth. from oxalic acid and $K_2[OsCl_6]$. Yellow. The corresp. chloro-bromo and chloro-iodo complexes, $[OsCl_nBr_{4-n}ox]^{2\ominus}$, $[OsCl_nI_{4-n}ox]^{2\ominus}$ are also known.

Di-Cs salt: [74335-03-8].

Bis-tetrabutylammonium salt: [74325-53-4].
Ir ν_{Os-Cl} 327 cm^{-1}.

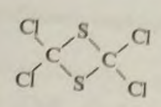
Homborg, H. *et al, Z. Naturforsch., B*, 1980, **35**, 554 (*synth, ir, uv, raman*)
Preetz, W. *et al, Z. Naturforsch., B*, 1981, **36**, 62 (*synth, ir, uv*)
Schulz, H. *et al, Z. Anorg. Allg. Chem.*, 1983, **502**, 66 (*use*)

$C_2Cl_4S_2$ IC-002894

2,2,4,4-Tetrachloro-1,3-dithietane, 9Cl

2,2,4,4-Tetrachloro-1,3-dithiacyclobutane. Dithiophosgene

[20464-23-7]



M 229.9

Interatomic distances: C—Cl 176-177.8, C—S 180.1 pm.

Synth. from CCl_2S + *hν*. Colourless cryst. (pet. ether and by subl.). Mp 119°. Dimer of Carbonothioic dichloride, IC-002354.

1-Oxide: [85989-11-3]. *2,2,4,4-Tetrachloro-1,3-dithietane-1-oxide*
$C_2Cl_4OS_2$ M 245.9
Synth. by oxidation of parent compd. with $F_3CCOOOH$ at 0°. Colourless cryst. (CH_2Cl_2/pet. ether). Sol. CH_2Cl_2. Mp 35°.

1,1-Dioxide: [73090-24-1]. *2,2,4,4-Tetrachloro-1,3-dithietane-1,1-dioxide*
$C_2Cl_4O_2S_2$ M 261.9
Synth. by oxidation of parent compd. with $KMnO_4$/HOAc. White cryst. (pet. ether or by subl.), dec. at 120° to C_2Cl_4. Sol. hexane. Mp 89.5°.

1,3-Dioxide: [85963-74-2].
Cryst. (MeCN). Mp 151°.

1,1,3-Trioxide: [85963-73-1].
$C_2Cl_4O_3S_2$ M 277.9
Synth. by oxidation of corresp. dioxide with $F_3CCOOOH$. Colourless cryst. Sol. CH_2Cl_2. Mp 107°.

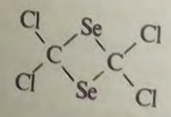
1,1,3,3-Tetraoxide: [57454-76-9].
$C_2Cl_4O_4S_2$ M 293.9
Synth. by oxidation of corresp. dioxide with CrO_3/HNO_3. Cryst. (pet. ether). Sol. hexane. Mp 200°. Bp 215°. Readily sublimes.

Schönberg, A. *et al, Chem. Ber.*, 1933, **66**, 567 (*synth*)
Jones, J.I. *et al, J. Chem. Soc.*, 1957, 614 (*ir, bibl*)
Busfield, W.K. *et al, Can. J. Chem.*, 1964, **42**, 2107 (*ir, raman*)
Krebs, B. *et al, Z. Naturforsch., B*, 1968, **23**, 741 (*synth, cryst struct*)
Seelinger, L. *et al, Angew. Chem., Int. Ed. Engl.*, 1980, **19**, 203 (*synth, ir, derivs*)
Balbach, B. *et al, Justus Liebigs Ann. Chem.*, 1980, 1981 (*oxides, cryst struct*)
Eschwey, M. *et al, Chem. Ber.*, 1983, **116**, 1623 (*derivs, synth, ir, ms, reactions*)

$C_2Cl_4Se_2$ IC-002895

2,2,4,4-Tetrachloro-1,3-diselenetane, 9Cl

[62247-73-8]



M 323.7

Formed from corresp. fluoro compd. + BCl_3 at 40°. Yellow-grey cryst., subl. *in vacuo*. Sol. $CHCl_3$. Bp 154-156°.

Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1976, **427**, 114 (*synth, ir, ms*)
Darmadi, A. *et al, Z. Naturforsch., B*, 1981, **36**, 1261 (*ir, raman, uv*)

C_2Cl_5F IC-002896

1,1,1,2,2-Pentachloro-2-fluoroethane

Fluorocarbon 111

[354-56-3]

M 220.2 Cl_3CCCl_2F

Cryoscopic solvent, refrigerant component. Solid with camphoraceous odour. d_{25} 1.74 (solid). Mp 101.3° (97°). Bp 138°.

▷ Production controlled by environmental legislation.

Booth, H.S. *et al, Ind. Eng. Chem.*, 1932, **24**, 328 (*synth, props*)
Bernstein, J. *et al, J. Am. Chem. Soc.*, 1940, **62**, 948 (*props*)
Rud Nielsen, J. *et al, J. Chem. Phys.*, 1953, **21**, 1070 (*ir, raman*)
Luft, N.W., *J. Phys. Chem.*, 1955, **59**, 92 (*props*)
Okuhara, K., *J. Org. Chem.*, 1978, **43**, 2745 (*synth, F-19 nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 861 (*props*)

C_2Cl_6 IC-002897

Hexachloroethane, 9Cl

Perchloroethane

[67-72-1]

M 236.7 Cl_3CCCl_3

Anthelmintic; used in pyrotechnics and chemical smokes, org. synth. Rhombohedra (EtOH/Et_2O). d_4^{20} 2.091. Bp 186.8° (triple point). Exists in 3 polymorphic forms.

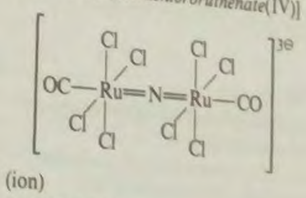
▷ Toxic, OES 50 mg m^{-3}. KI4025000.

Mkryan, G.M. *et al, CA*, 1943, **37**, 5694 (*synth*)
Calvez, Y. *et al, Helv. Chim. Acta*, 1974, **57**, 1433 (*synth*)
Hohlwein, D. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 2975; *Acta Crystallogr., Sect. A*, 1981, **37**, 904 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 780.
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 345.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1855.

$C_2Cl_8NO_2Ru_2^{3\ominus}$ IC-002898

Dicarbonyloctachloro-μ-nitridodiruthenate(3−), 9Cl

μ-Nitridobis[(carbonyl)tetrachlororuthenate(IV)]



M 555.7 (ion)

Tri-Cs salt: [42735-81-9].
$C_2Cl_8Cs_3NO_2Ru_2$ M 954.5
Prepd. by treating $[Ru_2NCl_8(OH_2)_2]^{3\ominus}$ in conc. HCl with CO, followed by CsCl. Brown salt; diamagnetic. Sol. aq. HCl. Ir ν_{CO} 2038; ν_{Ru_2N} 1016 cm^{-1}.

Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)

$C_2Cl_{10}NRe^{\ominus}$ IC-002899

Pentachloro[1,1,2,2,2-pentachloroethanaminato(2−)]rhenate(V)(1−), 10Cl

$[Cl_3CCCl_2N{\equiv}ReCl_5]^{\ominus}$

M 578.7 (ion)
Ir $\nu_{N\equiv C}$ 1241 cm^{-1}.
Ph_4As salt: [76130-52-4].
Synth. from $[Re(NC_2Cl_5)Cl_4(POCl_3)]$ and $AsPh_4Cl$ in CH_2Cl_2.

Dehnicke, K. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **469**, 45 (*synth, ir, struct, props*)

$C_2Cl_{10}NW^{\ominus}$ IC-002900

Pentachloropentachloroethylimidotungstate(V)
Pentachloro[1,1,2,2,2-pentachloroethanaminato(2−)]tungstate(V)(1−), 10Cl

$[Cl_3W{\equiv}N{-}CCl_2CCl_3]^{\ominus}$

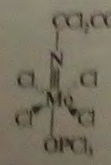
M 576.4 (ion)
W is six coordinate with W≡N 168 pm. Imide ligand exerts *trans*-influence: W—Cl_{trans} 242, W—Cl_{cis} 233 pm.
Ph_4As salt: [72902-16-0].
Synth. by action of $AsPh_4Cl$ on $POCl_3$ adduct of $Cl_3W{\equiv}NCCl_2CCl_3$. Red cryst. (MeCN). Less hygroscopic than starting material. Almost insol. CCl_4. Mp 205° (sealed tube). Ir $\nu_{W\equiv N}$ 1268 cm^{-1}.

Weiher, U. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **457**, 105 (*cryst struct, ir, synth*)

$C_2Cl_{12}MoNOP$ IC-002901

Tetrachloro(pentachloroethylimido)(phosphoryl trichloride)molybdenum(V)
Tetrachloro[1,1,2,2,2-pentachloroethanaminato(2−)](phosphoryl chloride-O)molybdenum(VI), 10Cl

[72451-93-5]



M 606.3
trans-Octahedral. Interatomic distances: Mo—N 169.2; Mo—O 221.7; Mo—Cl 229.6, 231.3, 231.8, 230.6pm. Synth. from $MoCl_5$ in $POCl_3$ + ClCN + Cl_3CCN. Green needles.

Dehnicke, K. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **456**, 71 (*cryst struct, synth, ir*)

$C_2Cl_{12}NOPRe$ IC-002902

Tetrachloro(pentachloroethylimido)(phosphoryl trichloride)rhenium(V)
Tetrachloro[1,1,2,2,2-pentachloroethanaminato(2−)](phosphoryl chloride-O)rhenium(VI), 10Cl

[73016-80-5]

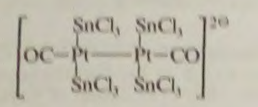
M 696.6
Octahedral.
trans-form
Interatomic distances: Re≡N 169, Re—O 218, Re—Cl 231.0 pm. Synth. from $ReCl_5$ dissolved in $POCl_3$ with CCl_3CN in the presence of Cl_2. V. hygroscopic, ochre-coloured cryst. Easily sol. $POCl_3$, CH_2Cl_2, $CHCl_3$, CCl_4.

Weiher, U. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **457**, 115 (*synth, cryst struct*)

$C_2Cl_{12}O_2Pt_2Sn_4^{2\ominus}$ IC-002903

Dicarbonyltetrakis(trichlorostannyl)diplatinate(2−), 11Cl

[102482-07-5]



M 1151.3 (ion)
Not isol. Obt. in soln. with $Bu_4N^{\oplus}$ as counterion.

Herbert, I.R. *et al*, *Inorg. Chim. Acta*, 1986, **112**, 29 (*synth, cmr, Sn-119 nmr, Pt-195 nmr*)

$C_2CoINO_3^{\ominus}$ IC-002904

Dicarbonyliodonitrosylcobaltate(1−), 8Cl

$[CoI(CO)_2NO]^{\ominus}$

M 271.8 (ion)
Reacts with benzyl halides to give benzaldoxime, PhCH=NOH.
Tetrabutylammonium salt: [33361-05-6].
Violet solid. Mp 73-75°. Ir ν_{CO} 2011, 1943, ν_{NO} 1712 cm^{-1} (diglyme).

Foa, M. *et al*, *J. Organomet. Chem.*, 1971, **30**, 123 (*synth, ir*)

C_2CoN_2 IC-002905

Cobalt(II) cyanide ($Co(CN)_2$)

[542-84-7]

$Co(CN)_2$

M 110.9
Struct. unknown. Blue cryst. powder. Insol. H_2O; sol. aq. KCN, aq. NH_3.
Dihydrate: [20427-11-6].
Pink solid.
Trihydrate: Red-grey powder. Sol. aq. KCN. Mp 250°.

Sidgwick, N.V. *et al*, *The Chemical Elements and their Compds.*, Oxford, 1950, 1380 (*synth, props*)
Poskozim, P.S. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 933 (*synth*)

C_2CoO_4 IC-002906

Cobalt(II) oxalate, 8Cl
Ethanedioic acid cobalt(2+) salt (1:1), 11Cl, 10Cl, 9Cl

[814-89-1]

$Co(C_2O_4)$

M 146.9
Exists in α and β modifications, β modification obt. by thermal dec. of dihydrate. Violet solid.
Dihydrate: [5965-38-8].
$C_2H_4CoO_6$ M 182.9
Commercially available. Pink solid. Sol. warm conc. NH_3, aq. $(NH_4)_2CO_3$.

[62782-24-5]
Remy, H., *Treatise on Inorg. Chem.*, Elsevier, 1956, **2**, 301 (*synth, props*)
Deyrieux, R. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 25 (*cryst struct, dihydrate*)
Pezerat, H. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 1000 (*cryst struct, dihydrate*)
Nikonenko, E.A. *et al*, *Zh. Neorg. Khim.*, 1982, **27**, 957; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 547 (*ir, uv-vis*)
Bogdanov, V.S. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 3063; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 1736 (*α,β forms*)
Kondrashev, Yu.D. *et al*, *Zh. Strukt. Khim.*, 1985, **26**, 90 (*cryst struct*)

C_2CrN_3 IC-002907

Chromium(II) cyanide ($Cr(CN)_2$), 10Cl

[79346-74-0]

$Cr(CN)_2$

M 104.0
Pale brown solid.
Dihydrate: [79346-47-7].
Dark green solid. Dehydrates at 100° *in vacuo*.

Eaton, J.P. *et al*, *Transition Met. Chem.*, 1981, **6**, 203 (*synth, ir, uv-vis, magnetism*)

C_2CrO_4 IC-002908

Chromium(II) oxalate
[Ethanedioato(2−)-O,O′]chromium

[89306-90-1]

$[Cr(C_2O_4)]_n$

M 140.0
Presumably polymeric with oxalato bridges and distorted octahedral coordination; usually said to be monohydrate. Yellow microcryst. Sol. hot H_2O, dil. acids. μ_{eff} = 4.5μ_B (340K); 4.0μ_B (100K).

Lux, H. *et al*, *Chem. Ber.*, 1958, **91**, 2143; 1959, **92**, 2364.
Earnshaw, A. *et al*, *Proc. Chem. Soc., London*, 1963, 281.
Aminov, T.G. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1965, **39**, 704; *CA*, **62**, 15576a.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1512 (*synth*)

$C_2Cs_2O_4$ IC-002909

Caesium oxalate
Dicaesium ethanedioate. Ethanedioic acid, dicaesium salt, 9Cl. Oxalic acid, dicaesium salt, 8Cl

[1068-63-9]

$Cs_2C_2O_4$

M 353.8
Synth. by passing CO through molten CsOH (above 300°) or by neutralisation of aq. CsOH with oxalic acid; cryst. as monohydrate. White powder. Dec. on heating → Cs_2CO_3. Extremely sol. H_2O (283 g per 100 cm^3 at 25°).
Monohydrate: [16799-57-8].
Cryst. from aq. solns. Colourless monoclinic cryst. Dec. on heating to form Cs_2CO_3.

Hackspill, L. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1948, **227**, 797 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 25, 1955, 241 (*hydrate, ir, Mössb*)
Peterson, R.F. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1498 (*hydrate, cryst struct, pmr*)

Simons, E.L. *et al*, *Talanta*, 1966, **13**, 199; *CA*, **64**, 10738f (*hydrate, synth*)
Kanamori, K., *Bull. Chem. Soc. Jpn.*, 1979, **52**, 2205 (*aq soln, raman*)

$C_2CuF_3O_2$ IC-002910

Trifluoroacetatocopper(I)
Acetic acid, copper(1+) salt, 9Cl. Copper(I) trifluoroacetate

[25535-55-1]

CF_3COOCu

M 176.5
Dimeric in the gas-phase. Tetrameric in solid state. Prepd. from Cu_2O + $(CF_3CO)_2O$. White needles.
Tetramer.
$C_8Cu_4F_{12}O_8$ M 706.2
Tetramer, bisbenzene complex: see *Tetrakis(trifluoroacetato)bis(benzene)tetracopper, IC-010328*

Ogura, T. *et al*, *Inorg. Chem.*, 1973, **12**, 2611 (*synth, mu*)
Kuyper, J. *et al*, *J. Organomet. Chem.*, 1975, **96**, 289 (*synth*)
Iijima, K. *et al*, *J. Mol. Struct.*, 1987, **158**, 315 (*mol struct, gas*)

$C_2CuN_3^{\ominus}$ IC-002911

Bis(cyano-C)cuprate(1−), 9Cl
Dicyanocuprate(1−)

[13682-73-0]

$[Cu(CN)_2]^{\ominus}$

M 115.5 (ion)
The anion forms helical chains with each copper atom 3-coordinate.
▷ GS2168900.
K salt: Copper potassium cyanide ($CuK(CN)_2$). *Cuprous potassium cyanide*
C_2CuKN_2 M 154.6
Used in electroplating. Cryst. (KCN aq.). Spar. sol. H_2O.

Basset, H. *et al*, *J. Chem. Soc.*, 1924, 1660.
Staritzky, E. *et al*, *Anal. Chem.*, 1956, **28**, 419 (*synth, cryst struct*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Interscience, New York, 1976, 266.
Merck Index, 11th Ed., 1989, 2672.

$C_2CuO_6^{2\ominus}$ IC-002912

Bis[carbonato(2−)-O]cuprate(II)(2−), 10Cl, 9Cl

[70948-67-3]

$[Cu(CO_3)_2]^{2\ominus}$

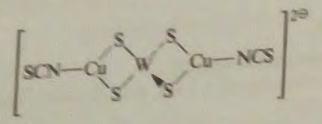
M 183.5 (ion)
Di-Na salt: [37224-64-9]. Copper(II) sodium carbonate ($CuNa_2(CO_3)_2$)
$C_2CuNa_2O_6$ M 229.5
Royal blue cryst. μ_{eff} = 1.92μ_B (100-400K). Struct comprises network of $[Cu(CO_3)_2^{2\ominus}]_n$ layers.
Di-K salt: [73949-69-6]. Copper(II) potassium carbonate ($CuK_2(CO_3)_2$)
$C_2CuK_2O_6$ M 261.7
3-D ferromagnet. Dark blue cryst. 3-D polymeric struct.

Appleby, M.P. *et al*, *J. Chem. Soc.*, 1918, **113**, 809 (*synth*)
Healy, P.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1913 (*cryst struct, deriv*)
Farrand, A. *et al*, *Aust. J. Chem.*, 1980, **33**, 431 (*cryst struct, deriv*)
Gregson, A.K. *et al*, *Inorg. Chem.*, 1981, **20**, 78; 1982, **21**, 3464 (*magnetism, synth, phys props*)

IC-002913

$C_2Cu_2N_2S_8W^{2\ominus}$

Tetra-μ-thioxobis[(thiocyanato-*N*)cuprate]tungstate(2−), 12CI



M 555.3 (ion)
Ir ν_{CN} 2100sh, 2088s, ν_{CS} 830m cm^{-1}.
Bis-Ph_4P salt: [111349-48-5].
Yellow cryst. Sol. Me_2CO, insol. heptane.
Potvin, C. *et al, Inorg. Chem.*, 1987, **26**, 4370 (*synth, cryst struct, ir*)

IC-002914

$C_2FN_2OPS_2$

Phosphorodi(isothiocyanatidic) fluoride, 9CI, 8CI
Fluorodiisothiocyanatooxophosphorus(V)
[14526-14-8]

$(SCN)_2P(O)F$

M 182.1
Highly reactive liq. $Bp_{3.5}$ 64-65°.
Roesky, H.W., *Chem. Ber.*, 1967, **100**, 2142 (*synth, F-19, P-31 nmr*)
Roesky, H.W., *Z. Anorg. Allg. Chem.*, 1967, **353**, 265 (*ir*)

IC-002915

$C_2FN_2O_2P$

Phosphorodiisocyanatidic fluoride, 9CI, 8CI
Fluorodiisocyanatooxophosphorus(V)
[17848-06-5]

$(OCN)_2P(O)F$

M 150.0
Highly reactive liq. d_4^{20} 1.60. Mp 144-146°. n_D^{20} 1.4160.
Derkach, G. *et al, Zh. Obshch. Khim.*, 1967, **37**, 2069; *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 1961 (*synth, ir*)

IC-002916

$C_2FO_6V^{2\ominus}$

Fluoro(oxalato)dioxovanadate(*V*)(2−)
[Ethanedioato(2−)-O,O′]fluorodioxovanadate(V)(2−), 9CI

M 189.9 (ion)
Trigonal bipyramidal.
Di-K salt: [53426-29-2].
Synth. as for NH_4 salt. Cryst.
Di-NH_4 salt: [53426-28-1].
Synth. from aq. HF soln. containing $H_2C_2O_4$, NH_4VO_3, $F^{\ominus}$ and $NH_4^{\oplus}$. Cryst.
Rieskamp, H. *et al, Z. Naturforsch., B*, 1974, **29**, 271 (*synth, ir, raman*)
Rieskamp, H. *et al, Z. Anorg. Allg. Chem.*, 1976, **419**, 193 (*cryst struct, NH_4 salt*)

IC-002917

C_2F_2

Difluoroacetylene
Difluoroethyne, 9CI
[689-99-6]

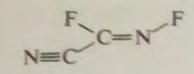
$FC{\equiv}CF$

M 62.0
Gas. Bp −15°. Polym. rapidly at r.t.
U.S. Pat., 2 831 835, (1958); *CA*, **52**, 14658f (*synth, props*)
Brahms, J.C. *et al, J. Am. Chem. Soc.*, 1989, **111**, 8940 (*synth, ir*)

IC-002918

$C_2F_2N_2$

Fluoro(fluoroimino)acetonitrile
Fluorocarbonocyanidimidic fluoride, 9CI
[14544-82-2]



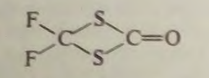
(Z)-form

M 90.0
Formed from N_2F_4 + $CFH{=}CH_2$ + CsF at 80° (via $F_2NCHFCH_2NF_2$). Colourless volatile liq.; isomers separated by glc.
Marsden, H.M. *et al, Inorg. Chem.*, 1987, **26**, 169 (*synth, ir, ms, F-19 nmr*)

IC-002919

$C_2F_2OS_2$

4,4-Difluoro-1,3-dithietan-2-one, 10CI
2,2-Difluoro-4-oxo-1,3-dithietane
[62982-88-1]



M 142.1
Minor product from reaction of 2,2,4,4-tetrachloro-1,3-dithietane + SbF_3. Colourless cryst. Mp 86°.
Diderrich, G. *et al, Chem. Ber.*, 1977, **110**, 916 (*synth, ir, F-19 nmr*)

IC-002920

$C_2F_3LiO_2$

Lithium trifluoroacetate
Lithium trifluoroethanoate. Trifluoroacetic acid, lithium salt, 8CI. Trifluoroethanoic acid, lithium salt
[2923-17-3]

$LiOOCCF_3$

M 119.9
Synth. from aq. Li_2CO_3 + F_3CCOOH. H_2O is removed initially by heating *in vacuo* using a steam bath and finally by azeotropic distillation using excess C_6H_6. Commercially available. When mixed with poly(ethylene oxide) it forms thin polymer electrolyte films which exhibit ionic conductivity. White powder.
▷ Irritant.
Jones, R.G. *et al, J. Am. Chem. Soc.*, 1973, **95**, 2465 (*synth, pmr*)
Regis, A. *et al, Chem. Phys. Lett.*, 1975, **32**, 462 (*ir in soln*)
Faniran, J.A. *et al, Spectrochim. Acta, Part A*, 1976, **32**, 1351 (*ir*)
White, E.V., *Org. Mass Spectrom.*, 1978, **13**, 495 (*ms*)
Tissot, P. *et al, Thermochim. Acta*, 1986, **106**, 377 (*thermal dec*)

IC-002921

C_2F_3N

Trifluoroisocyanomethane, 9CI
Trifluoromethyl isocyanide, 8CI
[19480-01-4]

$C{\equiv}NCF_3$

M 95.0
Synth. from $F_3CN{=}CBr_2$ + Mg in THF. Colourless gas, readily polym. to a yellow oil. Bp −80° (extrap.). Polymerises at pressure >200 mm Hg or in condensed phase.
Makarov, S.P. *et al, Zh. Obshch. Khim.*, 1967, **37**, 2781; *J. Gen. Chem. USSR (Engl. Transl.)*, 2667 (*synth*)
Banks, R.E. *et al, J. Chem. Soc. C*, 1969, 2119 (*synth*)
Lentz, D., *Ann. Chim. (Paris)*, 1984, **9**, 665 (*synth, bibl*)
Lentz, D., *Chem. Ber.*, 1984, **117**, 415 (*synth, reactions*)
Bock, H. *et al, Inorg. Chem.*, 1984, **23**, 1535 (*pe*)
Christen, D. *et al, J. Chem. Phys.*, 1984, **80**, 4020 (*ed*)
Lentz, D. *et al, J. Fluorine Chem.*, 1984, **24**, 523 (*synth, F-19 nmr, ir, ms*)
Lentz, D. *et al, Inorg. Chem.*, 1985, **24**, 4665 (*reactions*)

IC-002922

$C_2F_3O_4V$

Dioxo(trifluoroacetato-*O*)vanadium(*V*), 11CI
[37442-84-5]

$VO_2(OOCCF_3)$

M 195.9
Synth. from V_2O_5 and excess $(CF_3CO)_2O$ or from $VOCl_3$ andCF_3COOH. Yellow solid.
Radheshwar, P.V. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 3913 (*synth, ir*)
Puri, M. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1981, **11**, 539 (*synth, uv-vis, ir, magnetism*)

IC-002923

$C_2F_3O_5Re$

Trioxo(trifluoroacetato-*O,O′*)rhenium(*VII*), 11CI
Perrhenyl trifluoroacetate. (Trifluoroacetato) trioxorhenium(VII)

$ReO_3(O_2CCF_3)$

M 347.2
THF complex: [95458-12-1]. *Trioxo(tetrahydrofuran) (trifluoroacetato-O,O′)rhenium(VII)*
$C_6H_8F_3O_6Re$ M 419.3
Synth. from Re_2O_7 and $(CF_3CO)_2O$ in THF. Colourless, moisture sensitive cryst.; thermally unstable at r.t.
Edwards, P. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2695 (*synth, ir, nmr, props*)

IC-002924

C_2F_4

Tetrafluoroethylene
Tetrafluoroethene, 9CI. Fluorocarbon 1114. TFE
[116-14-3]

$F_2C{=}CF_2$

M 100.0
Manuf. by pyrolysis of $CHClF_2$. Used in manuf. of homo- and copolymers having valuable heat resistance, chemical inertness, electrical insulation and low friction props. Gas. Fp −142.5°. Bp −78.4°.
▷ Explodes under pressure, forms explosive peroxides, flammable. KX4000000.
Locke, E.G. *et al, J. Am. Chem. Soc.*, 1934, **56**, 1726.
Park, J.D. *et al, Ind. Eng. Chem.*, 1947, **39**, 354.
Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)
Venkateswarlu, Y. *et al, Chem. Process. Eng. (Bombay)*, 1970, **4**, 25 (*rev*)
Hunadi, R.J. *et al, Synthesis*, 1982, 454 (*synth*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 499
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3204.

IC-002925

$C_2F_4I_2$

1,1,2,2-Tetrafluoro-1,2-diiodoethane, 9CI
1,2-Diiodoperfluoroethane. sym-Diiodotetrafluoroethane
[354-65-4]

F_2ClCF_2I

M 353.8
d_4^{25} 2.629. Bp 112-113°, Bp_{14} 23°. n_D^{20} 1.489.
Kushida, K. *et al, Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co., 079 (*F-19 nmr*)
Emeleus, H.J. *et al, J. Chem. Soc.*, 1949, 2948 (*synth*)
Coffman, D.D. *et al, J. Org. Chem.*, 1949, **14**, 747 (*synth*)
Nodiff, E.A. *et al, J. Org. Chem.*, 1953, **18**, 235 (*props*)
Knunyants, I.L. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1964, 384 (*synth*)
Chung Wu, E. *et al, J. Phys. Chem.*, 1975, **79**, 1078 (*uv*)
Powell, D.L. *et al, J. Raman Spectrosc.*, 1978, **7**, 111 (*ir, raman*)
Ulm, K. *et al, Toxicol. Lett.*, 1980, **6**, 365 (*tox*)

IC-002926

$C_2F_4N_2$

(Difluoroamino)difluoroacetonitrile
[5131-88-4]

F_2NCF_2CN

M 128.0
Formed from N_2F_4 + $F_2C{=}CH_2$ + KF at 160°. Colourless gas. Adds 2ClF to C≡N.
Marsden, H.M. *et al, Inorg. Chem.*, 1987, **26**, 169 (*synth, ir, F-19 nmr*)

IC-002927

$C_2F_4N_2O_4$

1,1,2,2-Tetrafluoro-1,2-dinitroethane
[356-16-1]

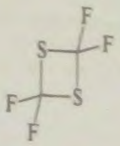
$O_2NCF_2CF_2NO_2$

M 192.0
d_4^{20} 1.608, d_4^{25} 1.602. Mp −41.5°. Bp 58-59° (65°). n_D^{25} 1.3265, n_D^{20} 1.3255.
[105159-88-4]
Haszeldine, R.N., *J. Chem. Soc.*, 1953, 2075 (*synth*)
Tetel'baum, B.I. *et al, Zh. Vses. Khim. Ova. im D.I. Mendeleeva*, 1963, **8**, 705 (*F-19 nmr*)
Fokin, A.V. *et al, Zh. Obshch. Khim.*, 1966, **36**, 119 (*synth*)

IC-002928

$C_2F_4S_2$

2,2,4,4-Tetrafluoro-1,3-dithietane, 9CI
[1717-50-6]



M 164.1

Source of Thiocarbonyl fluoride. IC-002407 by pyrolysis. Yellow liq. d_4^{20} 1.604. Mp −6°. Bp 48°. n_D^{25} 1.3908. δ_F +1.17($CFCl_2CFCl_2$), singlet.

1-Oxide: [85963-75-3].
$C_2F_4OS_2$ M 180.1
Formed from $(F_2CS)_2$ + F_2CCO_3H at 5°. Colourless liq. Bp 117° dec., Bp_{90} 60°. n_D^{20} 1.4415.

1,1-Dioxide: [767-45-3].
$C_2F_4O_2S_2$ M 196.1
Liq. Bp 105°. n_D^{25} 1.4108.

1,3-Dioxide: [75383-11-8]. *2,2,4,4-Tetrafluoro-1,3-dithietane-1,3-dioxide*
$C_2F_4O_2S_2$ M 196.1
Colourless cryst., dec. at 450° to unstable F_2CSO. Sol. Me_2CO.

1,1,3-Trioxide: [85963-76-4].
$C_2F_4O_3S_2$ M 212.1
Mp 81°.

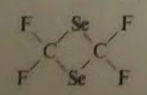
1,1,3,3-Tetroxide: [73090-23-0].
$C_2F_4O_4S_2$ M 228.1
Colourless cryst. Sol. CH_2Cl_2. Subl. 134°. Sensitive to hydrolysis.

Middleton, W.J. *et al, J. Org. Chem.*, 1965, **30**, 1375 (*synth*)
Long, R.C. *et al, J. Chem. Phys.*, 1971, **54**, 1563 (*pmr, cmr*)
Smith, Z. *et al, Acta Chem. Scand., Ser. A*, 1976, **30**, 759 (*ed*)
Chiang, J.F. *et al, J. Phys. Chem.*, 1977, **81**, 1682 (*ed*)
Klaboe, P. *et al, Spectrochim. Acta, Part A*, 1978, **34**, 789 (*ir, raman*)
Balbach, B. *et al, Justus Liebigs Ann. Chem.*, 1980, 1981 (*tetraoxide, cryst struct*)
Schomburg, D. *et al, J. Am. Chem. Soc.*, 1981, **103**, 406 (*dioxide, cryst struct*)
Eschwey, M. *et al, Chem. Ber.*, 1983, **116**, 1623 (*oxides, synth, ir, ms, F-19 nmr*)

$C_2F_4Se_2$ IC-002929

2,2,4,4-Tetrafluoro-1,3-diselenetane

[54393-42-9]



M 257.9
Formed by uv irradiation of F_2CSe or $(F_2CSe)_n$. Yellow cryst. Mp 38°.

Monomer: see *Selenocarbonyl difluoride, IC-002408*

Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1976, **427**, 114 (*synth, ir, ms, F-19 nmr, Se-77 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1978, **D6**, 250 (*bibl*)

$C_2F_5N_3O_2S_2$ IC-002930

Pentafluoro(imidosulfurous diisocyanato)sulfur, 10CI

[80044-07-1]

$(O{=}C{=}N)_2S{=}NSF_5$

M 257.1
Synth. from $F_3SN{=}SCl_2$ + AgNCO in C_6H_6 or from KOCN + $F_3SN{=}SCl_2$ + SO_2. Yellow liq., slowly dec. to F_3SNCO. Vp < 1 mm/25°.

Thrasher, J.S. *et al, J. Fluorine Chem.*, 1981, **18**, 537 (*synth, ir, ms, F-19 nmr*)

C_2F_6 IC-002931

Hexafluoroethane, 9CI

Fluorocarbon 116

[76-16-4]

F_3CCF_3

M 138.0
Dielectric. Gas. Fp −106.3° (−100.6°). Bp −79°. Non-flammable, non-toxic highly stable compd. Critical temp. 19.7°.

▷ KI4110000.

Swarts, F., *Bull. Soc. Chim. Belg.*, 1933, **42**, 114.
Ruff, O. *et al, CA*, 1933, **27**, 2131 (*synth*)
Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)

$C_2F_6FeO_6S_2$ IC-002932

Iron(*II*) trifluoromethanesulfonate

Ferrous trifluoromethanesulfonate. Ferrous triflate

[59163-91-6]

$Fe[OS(O)_2CF_3]_2$

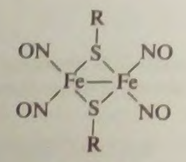
M 353.9
Synth. from anhyd. $FeCl_2$ + CF_3SO_3H. Catalyst for epoxidn. of olefins with iodosylbenzene. White hygroscopic powder. Sol. MeOH.

Haynes, J.S. *et al, Can. J. Chem.*, 1981, **59**, 669; 1986, **64**, 744 (*synth, magnetism, mössbauer*)

$C_2F_6Fe_2N_4O_4S_2$ IC-002933

Tetranitrosylbis(trifluoromethanethiolato)diiron, 9CI

[51059-38-2]



R = CF_3

M 433.8
Solid. Mp 51°. Sublimes.

Davidson, J.L. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1957 (*synth, ir, nmr*)

$C_2F_6HgS_2$ IC-002934

Bis(trifluoromethanethiolato)mercury, 9CI

Bis(trifluoromethylthio)mercury(II). *Mercury trifluoromethanethiolate*

[21259-75-6]

$F_3CSHgSCF_3$

M 402.7
Shiny plates with pungent odour. Sol. H_2O. Mp 39-40°. Subl. 65°.

Brandt, G.A.R. *et al, J. Chem. Soc.*, 1952, 2198 (*synth*)
Man, E.H. *et al, J. Am. Chem. Soc.*, 1959, **81**, 3575 (*synth, ir, uv, F-19 nmr*)
Downs, A.J. *et al, J. Chem. Soc.*, 1961, 3187 (*ir, raman, synth*)
Witel, K. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1975, **7**, 365 (*pe*)
Jubert, A.H. *et al, Can. J. Spectrosc.*, 1981, **26**, 207 (*ir, raman*)
Bierschenk, T.R. *et al, Inorg. Chem.*, 1982, **22**, 359 (*synth, F-19 nmr*)

$C_2F_6HgSe_2$ IC-002935

Bis(trifluoromethaneselenolato)mercury

Bis(trifluoromethylseleno)mercury. Bis[(trifluoromethyl)selenyl]mercury. Mercury trifluoromethylselenolate

[870-61-1]

$F_3CSeHgSeCF_3$

M 496.5
Monomeric in C_6H_6. Synth. from $(F_3C)_2Se_2$ + Hg in light. Pale yellow cryst. Sol. MeOH, CCl_4, Me_2O, C_6H_6. Mp 51°. Subl. 50° *in vacuo*.

[60129-77-3]

Marsden, C.J., *J. Fluorine Chem.*, 1975, **5**, 401, 423 (*nmr*)
Harris, R.K., *J. Phys. Chem.*, 1962, **66**, 768 (*nmr*)
Clase, H.J. *et al, J. Chem. Soc.*, 1965, 940 (*synth, ir, raman, uv*)
Birchall, T.J. *et al, Can. J. Chem.*, 1965, **43**, 1672 (*synth, Se-77 nmr*)
Dale, J.W. *et al, J. Chem. Soc.*, 1958, 2939 (*synth*)

$C_2F_6HgTe_2$ IC-002936

Bis(trifluoromethyltellurolato)mercury

Mercury trifluoromethyltelluride

[111053-35-1]

$F_3CTeHgTeCF_3$

M 593.8
Yellow powder. Sol. DMF, Me_2CO; insol. $CFCl_3$. Dec. at 77° to $(F_3C)_2Te_2$ and Hg.

Kischkewitz, J. *et al, Z. Anorg. Allg. Chem.*, 1987, **547**, 167 (*synth, ir, ms, F-19 nmr, thermal anal*)

$C_2F_6N_2S_3$ IC-002937

Bis[(trifluoromethyl)thio] sulfur diimide

Bis(trifluoromethylsulfenylimino)sulfane

[16489-12-6]

$F_3CSN{=}S{=}NSCF_3$

M 262.2
Formed from $F_3CSN{=}SF_2$ + F_3CSNH_2/NaF at 80° or by pyrol. of $(F_3CS)_3N$. Pale red liq. Mp −58°. Bp 142°.

Haas, A. *et al, Chem. Ber.*, 1968, **101**, 3407 (*synth, ir, uv*)
Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1974, **406**, 185 (*synth, ir, F-19 nmr*)

$C_2F_6NiO_6S_2$ IC-002938

Bis(trifluoromethanesulfonato)nickel(*II*)

Nickel(II) *triflate*

[60871-84-3]

$Ni(O_3SCF_3)_2$

M 356.8
Polymeric struct. with octahedral Ni. Prepd. by dehydration of $[Ni(H_2O)_6]^{2\oplus}$ $2CF_3SO_3^{\ominus}$. Yellow solid. Many complexes known, particularly with N ligands. Paramagnetic.

Janski, M.T. *et al, J. Inorg. Nucl. Chem.*, 1979, **41**, 1707 (*synth, uv, magnetism*)

$C_2F_6O_3$ IC-002939

Bis(trifluoromethyl) trioxide

[1718-18-9]

$F_3COOOCF_3$

M 186.0
Synth. from F_2CO + F_2O. Colourless gas. Stable in glass at 25°. Mp −138°. Bp −16°. Slowly hydrol. by H_2O. Dec. at 70° to O_2 + $(F_2C)_2O_2$.
▷ Highly toxic.

Inorg. Synth., 1970, **12**, 312 (*synth, F-19 nmr, ir*)

$C_2F_6O_6S_2Zn$ IC-002940

Bis(trifluoromethanesulfonato)zinc

Zinc trifluoromethylsulfonate. Zinc triflate

[54010-75-2]

$Zn(OSO_2CF_3)_2$

M 363.5
In aq. soln., the cation exists as $[Zn(OH_2)_6]^{2\oplus}$. Catalyst for dimerisation of acrylonitrile; for ethoxylation of butanol by ethylene oxide and for cationic polym. Solid + $2H_2O$ (H_2O). Sol. MeOH, EtOH, MeCN, DMF, formamide. The dihydrate is dehydrated at 120° at 0.2 mm. Stable up to 60°.

Hedwig, G.R. *et al, J. Am. Chem. Soc.*, 1974, **96**, 6589 (*synth*)
Takei, T., *Surf. Coat. Technol.*, 1985, **25**, 369 (*synth*)
Sperker, S. *et al, J. Solution Chem.*, 1988, **17**, 35 (*electrochem*)
Takei, T., *Surf. Coat. Technol.*, 1988, **35**, 57 (*progn*)

$C_2F_6O_7S_2V$ IC-002941

Oxobis(trifluoromethanesulfonato-*O*)vanadium(*IV*), 11CI

[63295-47-6]

$VO(OSO_2CF_3)_2$

M 365.0
Synth. from $VO(O_2CCF_3)_2$ and HSO_3CF_3 in CF_3COOH. Has been used as an accelerator in the hardening of epoxy resins by polyamines. Blue solid. Forms adducts with 2Py or bipy. Paramagnetic, μ_{eff} = 1.65μ_B. Ir $\nu_{V=O}$ 1024 cm^{-1}.

Ger. Pat., 2 647 377, (1977); *CA*, **87**, 54079x (*use*)
Sing, S. *et al, J. Fluorine Chem.*, 1985, **27**, 133 (*synth, thermal anal, ir, magnetism*)

C_2F_6S IC-002942

Bis(trifluoromethyl) sulfide

Thiobis[*trifluoromethane*]. *Hexafluorodimethyl sulfide*

[371-78-8]

$F_3C{-}S{-}CF_3$

M 170.0
Dielectric gas for high-voltage electrical apparatus. Gas. $d_4^{-63.5}$ 1.62. Mp < −119°. Bp −22.2°.

Brandt, G.R.A. *et al, J. Chem. Soc.*, 1952, 2198, 2549 (*synth, uv, ir*)
Bowen, H.J.M., *Trans. Faraday Soc.*, 1954, **50**, 452 (*ed*)
Harns, R.K., *J. Mol. Spectrosc.*, 1967, **10**, 309 (*F-19 nmr*)
Lawless, E.W. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 1541 (*synth, ir, F-19 nmr*)
Cullen, W.R. *et al, Inorg. Chem.*, 1970, **9**, 1976 (*ms, propn*)
Carter, H.A. *et al, Spectrochim. Acta, Part A*, 1973, **29**, 1479 (*raman*)
Zack, N.R. *et al, J. Fluorine Chem.*, 1975, **5**, 153 (*ms*)
De Marco, R.A. *et al, J. Magn. Reson.*, 1975, **18**, 522 (*cmr*)
Cowley, A.H. *et al, J. Am. Chem. Soc.*, 1979, **101**, 4074 (*pe*)
Oberhammer, H. *et al, J. Mol. Struct.*, 1981, **70**, 273 (*ir, raman, ed*)

C_2F_6S IC-002943

Trifluoroethylidynesulfur trifluoride

[88476-03-3]

$F_3CC{\equiv}SF_3$

M 170.0
Interatomic distances: F—C 132.9, C—C 145, C—S 143.4, S—F 156.1 pm; angle probably non linear: C—C≡S 155°. Formed from $CF_3CH{=}SF_4$ or $CF_3CH_2SF_3$ + KOH. Colourless as gas, liq. or solid. Mp −122.8°. Bp −15°. Forms cryst. dimer above −30°.

Dimer: $C_4F_{12}S_2$ M 340.1
Cryst.

Poetter, R. *et al, J. Am. Chem. Soc.*, 1985, **107**, 980 (*synth, ir, cmr, F-19 nmr, ms, cryst struct*)
Christen, D. *et al, J. Am. Chem. Soc.*, 1987, **109**, 4009 (*ir, raman, microwave*)

$C_2F_6S_2$ IC-002944

Bis(trifluoromethyl) trisulfide

[372-06-5]

$F_3C{-}S{-}S{-}S{-}CF_3$

M 234.2
Bp 86.4°; n_D^{20} 1.4023. Stable to air, water and mercury at r.t.

Haszeldine, R.N. *et al, J. Chem. Soc.*, 1953, 3219 (*synth, ir, uv*)
Bowen, H.J.M., *Trans. Faraday Soc.*, 1954, **50**, 452 (*ed*)
Cullen, W.R. *et al, Inorg. Chem.*, 1969, **8**, 1803 (*props*)
Zack, N.R. *et al, J. Fluorine Chem.*, 1975, **5**, 153 (*ms*)
Gombler, W. *et al, Z. Naturforsch., B*, 1975, **30**, 169 (*ms, F-19 nmr*)
Yasumura, T. *et al, Inorg. Chem.*, 1978, **17**, 3108 (*synth, ir, ms, F-19 nmr*)

$C_2F_6S_4$ IC-002945

Bis(trifluoromethyl) tetrasulfide

[372-07-6]

$F_3C{-}S{-}S{-}S{-}S{-}CF_3$

M 266.2
Bp 135° n_D^{20} 1.4608. Stable to air, water, and mercury at r.t.

Haszeldine, R.N. *et al, J. Chem. Soc.*, 1953, 3219 (*synth, ir, uv*)
Cullen, W.R. *et al, Inorg. Chem.*, 1969, **8**, 1803 (*props*)
Gombler, W. *et al, Z. Naturforsch., B*, 1975, **30**, 169 (*ms, F-19 nmr*)
Yasumura, T. *et al, Inorg. Chem.*, 1978, **17**, 3108 (*synth, ir, ms, F-19 nmr*)

C_2F_6Se IC-002946

Bis(trifluoromethyl)selenium

Selenobis[trifluoromethane], 10Cl. Bis(trifluoromethyl)selane

[371-79-9]

$Se(CF_3)_2$

M 216.9
Formed from $SeBr_4$ + $Hg(CF_3)_2$ at 210°. Colourless gas. Sol. org. solvs. Bp −2°.

Dale, J.W., *J. Chem. Soc.*, 1958, 2939 (*synth*)
Ganja, E.A., *Inorg. Chem.*, 1988, **27**, 4535 (*synth, ms, nmr*)

$C_2F_6Se_2$ IC-002947

Bis(trifluoromethyl)diselenium

Bis(trifluoromethyl) diselenide, 10Cl. Bis(trifluoromethyl) diselane. 1,1,1,4,4,4-Hexafluoro-2,3-diselenabutane

[372-65-6]

$F_3CSeSeCF_3$

M 295.9
Formed from $SeBr_4$ + $Hg(CF_3)_2$ at 170°. Yellow liq., involatile at −116°. Sol. org. solvs. Bp 70°.

Dale, J.W., *J. Chem. Soc.*, 1958, 2939 (*synth*)
Ganja, E.A., *Inorg. Chem.*, 1988, **27**, 4535 (*synth, ms, nmr*)

C_2F_6Te IC-002948

Bis(trifluoromethyl)tellurium

Tellurobis[trifluoromethane], 9Cl. Bis(trifluoromethyl)tellane

[55642-42-7]

$Te(CF_3)_2$

M 265.6
Formed from $TeBr_4$ + $Hg(CF_3)_2$ at 155°. Yellow gas, involatile at −116°. Sol. org. solvs. Mp < −160°. Bp −98°.

Lagow, R.J. *et al, J. Am. Chem. Soc.*, 1975, **97**, 518 (*synth, ir, F-19 nmr*)
Juhlke, T.J. *et al, J. Am. Chem. Soc.*, 1979, **101**, 3229 (*synth, F-19 nmr*)
Ganja, E.A. *et al, Inorg. Chem.*, 1988, **27**, 4535 (*synth, ms, nmr*)

$C_2F_6Te_2$ IC-002949

Bis(trifluoromethyl)ditellurium

Bis(trifluoromethyl) ditelluride, 10Cl. Bis(trifluoromethyl) ditellane. 1,1,1,4,4,4-Hexafluoro-2,3-tellurabutane

[1718-20-3]

$F_3CTeTeCF_3$

M 393.2
Synth. from Te + $CF_3^{\cdot}$. Red liq. Stable to air and H_2O. Thermally unstable. Hydrol. by $OH^{\ominus}$. Sol. org. solvs. Insol. H_2O. Mp −73°. Bp −53°.

Bell, T.N. *et al, Aust. J. Chem.*, 1963, **16**, 722 (*synth*)
Lagow, R.J. *et al, J. Am. Chem. Soc.*, 1975, **97**, 518 (*synth, ir, ms, F-19 nmr*)
Juhlke, T.J. *et al, J. Am. Chem. Soc.*, 1979, **101**, 3229 (*synth, F-19 nmr*)

C_2F_6Xe IC-002950

Bis(trifluoromethyl)xenon

[72599-34-9]

$(F_3C)_2Xe$

M 269.3
Formed from XeF_2 + $CF_3^{\cdot}$. Volatile white solid at −78°. Highly unstable, $t_{\frac{1}{2}}$ ~ 30 min at 25°; ~ 2 weeks at −196°. Dec. by O_2, H_2O, glass. Dec. at 20° to XeF_2 + mixed fluorocarbons.

Turbini, L.J. *et al, J. Am. Chem. Soc.*, 1979, **101**, 5833 (*synth, ms, ir, F-19 nmr*)

C_2F_8Ge IC-002951

Difluorobis(trifluoromethyl)germane

Bis(trifluoromethyl)germanium(IV) *fluoride*

[56592-86-0]

$(F_3C)_2GeF_2$

M 248.6
Mp 49.2°. Subl. 32°.

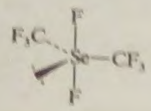
Eujen, R. *et al, J. Organomet. Chem.*, 1975, **88**, 165 (*synth, F-19 nmr*)
Buerger, H. *et al, Spectrochim. Acta, Part A*, 1975, **31**, 1655 (*ir, raman*)
Eujen, R. *et al, J. Fluorine Chem.*, 1983, **22**, 263 (*synth, F-19 nmr*)

C_2F_8Se IC-002952

Difluorobis(trifluoromethyl)selenium

Bis(trifluoromethyl)selenium difluoride

[59802-61-8]



M 254.9
Interatomic distances: F—Se 182.7, Se—C 202.2, C—F 131.4 pm; angles: CSeC 118.7°, FSeF 157.8°. Synth. from AgF_2 or XeF_2 + $(F_3C)_2Se$. Colourless liq. Reacts with glass forming $(F_3C)_2SeO$. Mp −15°.

Lau, C. *et al, J. Fluorine Chem.*, 1976, **7**, 261 (*synth, ms, ir, F-19 nmr*)
Baxter, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 941 (*synth, ed*)

C_2F_8Te IC-002953

Trifluoro(pentafluoroethyl)tellurium

Perfluoroethyltellurium trifluoride

[51255-75-5]

$F_3CCF_2TeF_3$

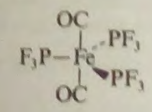
M 303.6
Translucent cryst. Mp 142-143°. Tetrahedral.

Desjardins, C.D. *et al, Inorg. Nucl. Chem. Lett.*, 1974, **10**, 151 (*synth, F-19 nmr*)
Lau, C. *et al, Can. J. Chem.*, 1985, **63**, 2273 (*synth, raman, cryst struct, F-19 nmr*)

$C_3F_6FeO_2P_3$ IC-002954

Dicarbonyltris(phosphorous trifluoride)iron

[17594-26-2]



trans-form

M 375.7
Exists as mixt. of 3 rapidly equilibrating isomers (*cis*, *trans*, and *vic*-forms). V. volatile yellow liq., unstable towards air and water. Sol. cyclohexane, C_6H_6, attacked rapidly by Me_2CO, EtOH. Immisc. H_2O. Most volatile component of series $(CO)_{5-n}Fe(PF_3)_n$.

Clark, R.J. *et al, Inorg. Chem.*, 1964, **3**, 1395 (*synth*)
Haas, H. *et al, J. Chem. Phys.*, 1967, **47**, 2996 (*ir*)
Udovich, C.A. *et al, Inorg. Chem.*, 1969, **8**, 1066 (*stereochem*)
Clark, R.J. *et al, Acc. Chem. Res.*, 1973, **6**, 246 (*rev*)
Sheline, R.K. *et al, New Synth. Methods*, 1975, **3**, 219 (*ir, nmr*)
Mahnke, H. *et al, J. Chem. Phys.*, 1977, **66**, 4822 (*cmr, ir*)
Head, R.A. *et al, J. Organomet. Chem.*, 1978, **145**, 75 (*pe*)

$C_3F_6O_3P_3Ru$ IC-002952 – IC-002960

Dicarbonyltris(phosphorous trifluoride)ruthenium, 9Cl

[36430-00-9]

$Ru(CO)_3(PF_3)_3$

M 420.9
May be a fluxional isomeric mixt. Isol. from autoclave reaction of CO + PF_3 + $Ru_3(CO)_{12}$. Light-yellow liq. Ir ν_{CO} 2078, 2038, 2026, 2007 cm^{-1} (hexane).

Udovich, C.A. *et al, J. Organomet. Chem.*, 1972, **36**, 355 (*synth, ir, nmr, ms*)

$C_2F_{10}S$ IC-002956

Pentafluoro(pentafluoroethyl)sulfur

Pentafluoroethylsulfur pentafluoride

[354-67-6]

$F_3CCF_2SF_5$

M 246.0
Bp 13.4-14.2° (11.3°). Octahedral struct.

Dresdner, R.D. *et al, J. Am. Chem. Soc.*, 1959, **81**, 574 (*synth*)
Rogers, M.T. *et al, J. Am. Chem. Soc.*, 1962, **84**, 3666 (*F-19 nmr*)
Abe, T. *et al, J. Fluorine Chem.*, 1973, **3**, 187 (*synth, F-19 nmr*)

$C_2F_{10}S$ IC-002957

Tetrafluorobis(trifluoromethyl)sulfur(*VI*)

Bis(trifluoromethyl)sulfur tetrafluoride

$(F_3C)_2SF_4$

M 246.0
Liq. or gas. Bp 20°. Isomeric form not reported.

[42179-02-2, 42179-03-3]

Clifford, A.F. *et al, J. Chem. Soc.*, 1953, 2372 (*synth, ir, props*)
Young, J.A. *et al, J. Org. Chem.*, 1959, **24**, 1021 (*synth, F-19 nmr*)
Abe, T. *et al, J. Fluorine Chem.*, 1973, **3**, 187 (*F-19 nmr*)

$C_2F_{12}S_2$ IC-002958

[μ-(2,2-Difluoroethenediyl)]decafluorodisulfur

1,1-Difluoro-2,2-bis(pentafluorosulfur)ethene

[117146-24-4]

$(F_5S)_2C{=}CF_2$

M 316.1
Formed from $(F_5S)_2CHCF_2Cl$ + KOH. Colourless liq. Bp 88°.

Gerhardt, R. *et al, Angew. Chem., Int. Ed. Engl.*, 1988, **27**, 1534 (*synth, F-19 nmr, ir, ms*)

C_2FeIO_2 IC-002959

Dicarbonyliodoiron(*I*)

$Fe(CO)_2I$

M 238.7

Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1940, **245**, 295 (*synth*)

$C_2FeI_2O_2$ IC-002960

Dicarbonyldiiodoiron(*II*)

$Fe(CO)_2I_2$

M 365.6
Prepd. from $Fe_2(CO)_8I_2$.

Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1932, **204**, 174; 1940, **245**, 295 (*synth*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1967, **6**, 2113 (*synth, ir*)

IC-002961

C_2FeN_2

Iron(*II*) cyanide ($Fe(CN)_2$)
Ferrous cyanide. Ferrous ferrocyanide. Iron(II) *hexacyanoferrate*(II)
[1948-47-6]

$Fe_2[Fe(CN)_6]$

M 107.8
Compd. has empirical formula $Fe(CN)_2$ but is probably $Fe_2[Fe(CN)_6]$. Obt. on heating $H_4Fe(CN)_6$ or $(NH_4)_4[Fe(CN)_6]$. Has hydrometallurgical applications. Pale green or yellow powder. Forms $Fe(OH)_2$ and $K_4[Fe(CN)_6]$ with aq. KOH.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, **B**, 560 (*rev, bibl*)

IC-002962

$C_2FeN_2O_4$

Dicarbonyldinitrosyliron, 9CI, 8CI
[13682-74-1]

$Fe(CO)_2(NO)_2$

M 171.8
Tetrahedral. Deep-red, volatile cryst., unstable to air. Somewhat unstable above 0°. Sol. org. solvs.; insol. H_2O. Mp 18.5°. Subl. easily.

Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1932, **208**, 238; 1963, **320**, 101 (*synth*)
Brockway, L.O. *et al*, *Trans. Faraday Soc.*, 1937, **33**, 1233 (*struct*)
McBride, D.W. *et al*, *Inorg. Chem.*, 1962, **1**, 386 (*synth*)
Organomet. Synth., 1965, **1**, 167 (*synth*)
Bramley, R. *et al*, *J. Chem. Soc. A*, 1967, 861 (*cmr*)
Poletti, A. *et al*, *Inorg. Chim. Acta*, 1968, **2**, 157 (*ir*)
Mossbaek, H. *et al*, *Acta Chem. Scand., Ser. A*, 1974, **28**, 157 (*mössbauer*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1984 (*synth*)
Paliani, G. *et al*, *Can. J. Spectrosc.*, 1976, **21**, 159 (*ir*)
Chen, H.W. *et al*, *Inorg. Chem.*, 1979, **18**, 2548 (*synth, pe*)
Jenny, T. *et al*, *J. Organomet. Chem.*, 1981, **205**, 211 (*nmr*)
Hedberg, L. *et al*, *Inorg. Chem.*, 1985, **24**, 2766 (*ed*)
Godd, G.E. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2547 (*ir*)

IC-002963

C_2FeO_4

Iron(*II*) oxalate
Ferrous oxalate. Ferrous ethanedioate. Iron(II) *ethanedioate. Oxalic acid, iron*(2+) *salt*
[516-03-0]

$Fe(C_2O_4)$

M 143.8
Fe(*II*) octahedrally coord. to two bidentate $[C_2O_4]^{2\ominus}$ and 2 bridging $[C_2O_4]^{2\ominus}$. Component of coatings for cold forming of alloy steels. Corrosion inhibitor; heat stabiliser; catalyst. Commercially available as dihydrate. Solid.

[6047-25-2]

*Gmelin Handbook Inorg. Chem., Syst. No.*59, 1930, **B**, 532 (*bibl, rev*)
Waterman, V., *J. Org. Chem.*, 1949, **14**, 289 (*synth*)
Figgis, B.N. *et al*, *Prog. Inorg. Chem.*, 1964, **6**, 177 (*magnetism*)
Nikonenko, E.A. *et al*, *Zh. Neorg. Khim.*, 1982, **27**, 975 (*struct*)
Ramani, S. *et al*, *Mater. Chem. Phys.*, 1983, **9**, 539 (*thermal dec, mössbauer*)
Jiingyann, C. *et al*, *J. Appl. Phys.*, 1985, **57**, 3338 (*magnetism*)
Kondrashev, Yu.D. *et al*, *Zh. Strukt. Khim.*, 1985, **26**, 90 (*struct*)

IC-002964

$C_2HBrClF_3$

2-Bromo-2-chloro-1,1,1-trifluoroethane, 9CI
***Halothane*, BAN, INN.** *Fluorocarbon 123B1. Alotano. Anestan. Fluothane. Ftorotan. Halan. Halovis. Narcotan. Somnothan. Trothane*
[151-67-7]

$HBrClCCF_3$

M 197.3
Manuf. by bromination of CF_3CH_2Cl. Inhalation anaesthetic. Spar. sol. H_2O. d_4^{20} 1.86. Bp 50.2°. Light sensitive.

▷ Exp. teratogen. KH6550000.

Raventós, J., *Br. J. Pharmacol.*, 1956, **11**, 394.
Daley, R.D. *et al*, *Anal. Profiles Drug Subst.*, 1972, **1**, 119; 1973, **2**, 573; 1985, **14**, 597 (*revs*)
Ngai, S.H., *Handb. Exp. Pharmacol.*, Springer-Verlag, Berlin, 1972, **30**, 33 (*rev*)
Dobkin, A.B., *Monogr. Anaesthesiol.*, 1979, **6**, 59 (*rev, pharmacol*)
Smith, G., *Br. J. Anaesth.*, 1981, **53**, 17 (*use*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 3101.
Torri, G. *et al*, *Prog. Anesthesiol.*, 1983, **3**, 141 (*rev, metab*)
Neuberger, J. *et al*, *Br. Med. J.*, 1984, **289**, 1136 (*tox*)
Stock, J.G.L. *et al*, *Anesthesiology*, 1985, **63**, 424 (*rev, tox*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1835.

IC-002965

C_2HBrF_4

2-Bromo-1,1,1,2-tetrafluoroethane, 9CI, 8CI
***Teflurane*, USAN, INN.** *Terflurane. Abbott 16900. DA 708. Fluorocarbon 124B1*
[124-72-1]

$F_3CCHFBr$

M 180.9
(±)-*form*
Inhalatory anaesthetic. Gas. Bp 8°. Nonexplosive, nonflammable.

Rausch, D.A. *et al*, *J. Org. Chem.*, 1963, **28**, 494 (*synth*)
Millar, R.A. *et al*, *Br. J. Anaesth.*, 1970, **42**, 366 (*pharmacol*)
Black, G.W. *et al*, *Int. Anesthesiol. Clin.*, 1971, **9**, 171 (*rev, pharmacol*)
Seyferth, D. *et al*, *J. Organomet. Chem.*, 1975, **92**, 7 (*synth*)

IC-002966

C_2HClF_2

1-Chloro-1,2-difluoroethene, 9CI
Fluorocarbon 1122a
[359-04-6]

$FClC{=}CHF$

M 98.4
Bp −15° to −12° (−6° to −4°). Prob. mixt. of geom. isomers.

▷ KU9900000.

[2837-86-7, 27156-04-3, 30860-28-7]

Birchall, J.M. *et al*, *J. Chem. Soc.*, 1961, 2204 (*synth*)
Fuller, G. *et al*, *Tetrahedron*, 1962, **18**, 123 (*synth*)
Barlow, M.G., *J. Chem. Soc., Chem. Commun.*, 1966, 703 (*F-19 nmr*)

Craig, N.C. *et al*, *J. Phys. Chem.*, 1971, **75**, 1453 (*isom*)
Syrvatka, B.G. *et al*, *Zh. Org. Khim.*, 1972, **8**, 1553 (*ms*)
Ruehl, E., *Can. J. Chem.*, 1985, **63**, 1949 (*uv*)

IC-002967

C_2HClF_2

2-Chloro-1,1-difluoroethene, 9CI
2,2-Difluorovinyl chloride. 1-Chloro-2,2-difluoroethylene. Fluorocarbon 1122
[359-10-4]

$F_2C{=}CHCl$

M 98.4
Gas. Mp −138.5°. Bp −19.0° (−17.7°).

▷ Flammable, toxic. KU9920000.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 1025 (*synth*)
Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)
Chandra, S., *J. Phys. Chem.*, 1967, **71**, 1927 (*microwave*)
Torkelson, T.R. *et al*, *Toxicol. Appl. Pharmacol.*, 1971, **19**, 1 (*tox*)
Scott, J.D. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2634 (*uv*)
Mackenzie, M.W., *Spectrochim. Acta, Part A*, 1984, **40**, 279 (*ir*)
Osten, H.J. *et al*, *J. Chem. Phys.*, 1985, **83**, 5434 (*F-19 nmr*)

IC-002968

C_2HClF_3N

***N*-(Trifluoromethyl)chloroformimide**
N-(Trifluoromethyl)chloromethanimine, 11CI
[99298-38-1]

$F_3CN{=}CHCl$

M 131.4
Synth. from $F_3CN{\equiv}C$ + HCl at 20°. Colourless liq. Bp 27°.

[99298-39-2]

Lentz, D. *et al*, *Inorg. Chem.*, 1985, **24**, 4665 (*synth, ir, raman, ms, pmr, F-19 nmr, ed*)

IC-002969

C_2HClF_4

1-Chloro-1,1,2,2-tetrafluoroethane
Fluorocarbon 124a
[354-25-6]

$F_2CClCHF_2$

M 136.4
Propellant, working fluid for Rankine cycle pumps. Refrigerant component with low ozone depletion potential. d_4^{20} 1.379. Mp −117°. Bp −10.2°, Bp −13°.

[63938-10-3]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 402 (*synth*)
Cuculo, J.A. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 710 (*synth*)
Klaboe, P. *et al*, *J. Chem. Phys.*, 1961, **34**, 1819 (*ir, raman*)
Smart, B.E., *Kirk-Othmer Encycl. Chem. Technol.*, 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 861 (*props*)

IC-002970

C_2HClF_4

2-Chloro-1,1,1,2-tetrafluoroethane
Fluorocarbon 124
[2837-89-0]

$F_3CCHClF$

M 136.4
(±)-*form*
Working fluid for heat pumps, blowing agent, propellant, solvent for degreasing and defluxing substrates. Bp −8° (−12°).

▷ OES 1000 ppm -fv/v. Shows anaesthetic props.

[63938-10-3]

Miller, W.T. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 3091 (*synth*)
Goldwhite, H. *et al*, *J. Chem. Soc.*, 1961, 3825 (*synth, ir*)
Noftle, R.E. *et al*, *J. Fluorine Chem.*, 1984, **26**, 29 (*ir, raman*)

IC-002971

C_2HCl_2F

1,1-Dichloro-2-fluoroethene, 9CI
Fluorocarbon 1121a
[359-02-4]

$Cl_2C{=}CHF$

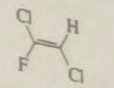
M 114.9
d_4^{20} 1.383. Mp −108.8°. Bp 37-39°. n_D^{20} 1.4036.

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 402 (*synth*)
Yanwood, J., *J. Chem. Soc.*, 1965, 7481 (*ir, raman*)
Craig, N.C., *J. Mol. Spectrosc.*, 1967, **23**, 307 (*ir, raman*)
Moehlmann, J.G. *et al*, *J. Chem. Phys.*, 1975, **62**, 3052 (*synth, ir*)

IC-002972

C_2HCl_2F

1,2-Dichloro-1-fluoroethene, 9CI
Fluorocarbon 1121
[430-58-0]



M 114.9
(*E*)-*form*
(*E*)-*form* [13245-54-0]
Mp −114.8°. Bp 37.5°.
(*Z*)-*form* [13245-53-9]
Mp −116.1°. Bp 31.0°.
[27156-05-4]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 402 (*synth*)
Craig, N.C. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 3232 (*synth, ir, raman, pmr*)
Bell, C.L. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 2344 (*pmr, F-19 nmr*)
Craig, N.C. *et al*, *J. Mol. Spectrosc.*, 1967, **23**, 307 (*ir, raman*)
Jeffers, P.M., *J. Phys. Chem.*, 1974, **78**, 1469 (*isom*)

IC-002973

$C_2HCl_2F_3$

1,1-Dichloro-1,2,2-trifluoroethane, 9CI
Fluorocarbon 123b
[812-04-4]

Cl_2CFCF_2H

M 152.9
Bp 59-61°, Bp 30.2°.

Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1960, 4503 (*synth*)
Fuller, G. *et al*, *Tetrahedron*, 1962, **18**, 123 (*synth*)

IC-002974

$C_2HCl_2F_3$

1,2-Dichloro-1,1,2-trifluoroethane, 9CI
Fluorocarbon 123a
[354-23-4]

$F_2CClCHClF$

M 152.9
Refrigerant. Liq. $d_4^{27.4}$ 1.498. Bp 28-30°. n_D^{15} 1.3371.

▷ Irritant, convulsant, shows anaesthetic props. KI1106000.

[34077-87-7, 90454-18-5]

Glockler, G. *et al*, *J. Chem. Phys.*, 1941, **9**, 387 (*raman*)
Park, J.D. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 711 (*synth, ir*)
Fuller, G. *et al*, *Tetrahedron*, 1962, **18**, 123 (*tox*)
Doucet, J. *et al*, *J. Chem. Phys.*, 1975, **62**, 355 (*uv, pe*)

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 861 (*props*)
Capnel, P. *et al*, *Tetrahedron*, 1979, **35**, 2661 (*F-19 nmr*)
Service, C.F. *et al*, *J. Fluorine Chem.*, 1982, **20**, 135 (*synth*)

IC-002975

$C_2HCl_2F_3$

2,2-Dichloro-1,1,1-trifluoroethane, 9CI
Fluorocarbon 123. HCFC 123
[306-83-2]

F_3CCHCl_2

M 152.9
Refrigerant, degreasing solvent. Potential replacement for Fluorocarbon 11 with low ozone depletion capacity. Liq. d_4^{15} 1.475. Mp −107°. Bp 28.7°, Bp_{747} 27.1°. pK_a 17.2 (37°). n_D^{15} 1.333.

▷ Shows anaesthetic props., suspect carcinogen. KI1108000.

McBee, E.T. *et al*, *Ind. Eng. Chem.*, 1947, **39**, 409 (*synth*)
Nielsen, J.R. *et al*, *J. Chem. Phys.*, 1953, **21**, 1060 (*ir, raman*)
Ng, S., *J. Magn. Reson.*, 1972, **7**, 370 (*pmr*)
Burns, T.H.S. *et al*, *Anaesthesia*, 1982, **37**, 278 (*use*)
Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co., 1988, 016, 017 (*F-19 nmr, pmr*)

IC-002976

C_2HCl_3

Trichloroethylene, 8CI, INN
Trichloroethene, 9CI. Tri-Clene. Trichloran. Chlorylen. R 1120. Other proprietary names
[79-01-6]

$Cl_2C{=}CHCl$

M 131.3
Manuf. by treatment of tetrachloroethane with strong base. Industrial solv. for grease, waxes, oils, paints and adhesives etc.; veterinary inhalation anaesthetic. Used in manuf. of fluorocarbons. Nonflammable mobile liq. with characteristic odour. Insol. H_2O, sol. most org. solvs. d_4^{20} 1.46. Mp −84.8° (−86.8). Bp 86.7°, Bp_{60} 20.0°.
Widespread use declining due to toxicity.

▷ Mod. toxic by inhalation and skin absorption, OES 420 mg m^{-3} (max. exp. limit). Violent reacn. with many metals. Vapour can ignite or explode if heated. KX4550000.

Japan. Pat., 6874, (1954); *CA*, **50**, 2651 (*synth*)
Shikaji, T., *Chem. Eng. (London)*, 1970, **77**, 74 (*synth*)
Waters, E.M. *et al*, *J. Toxicol. Environ. Health*, 1977, **2**, 671 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 745 (*rev*)
Fielder, R.J. *et al*, *Toxic. Rev.*, 1982, 6 (*rev, metab, tox*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 32.
Bretherick, L., *Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91 (*haz*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 514.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3329.

IC-002977

$C_2HCl_3F_2$

1,1,1-Trichloro-2,2-difluoroethane
Fluorocarbon 122b
[354-12-1]

Cl_3CCHF_2

M 169.3
Photoresist. remover for printed circuits and semiconductors. Developer for resists. Dry cleaning solvent. Liq., glass at low temp. d_4^{20} 1.566. Bp 73°.

[41834-16-6]

Heberling, J.W., *J. Org. Chem.*, 1958, **23**, 615.
Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1960, 4503 (*synth*)

IC-002978

$C_2HCl_3F_2$

1,1,2-Trichloro-1,2-difluoroethane, 9CI
Fluorocarbon 122a
[354-15-4]

$Cl_2CFCHFCl$

M 169.3
d_4^{20} 1.559. Bp 71-72.6°. n_D^{20} 1.3942 (1.3967).

▷ Shows anaesthetic props.

Hauptschein, M. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3423 (*synth*)
Bindal, M.C. *et al*, *Arzneim.-Forsch.*, 1980, **30**, 234 (*use, ir*)

IC-002979

$C_2HCl_3F_2$

1,2,2-Trichloro-1,1-difluoroethane, 9CI
Fluorocarbon 122
[354-21-2]

$F_2CClCHCl_2$

M 169.3
Liq. Mp −140°. Bp 71.9°.

▷ Shows anaesthetic props.. KI1435000.

[41834-16-6]

Heberling, J.W., *J. Org. Chem.*, 1958, **23**, 615 (*synth, ms*)
Fessenden, R.W. *et al*, *J. Chem. Phys.*, 1962, **37**, 1466 (*pmr, F-19 nmr*)
Hørnischer, R. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 81 (*raman*)
Chuvatken, N.N. *et al*, *Zh. Org. Khim.*, 1982, **18**, 946 (*synth*)

IC-002980

C_2HCl_4F

1,1,1,2-Tetrachloro-2-fluoroethane, 9CI
Fluorocarbon 121a
[354-11-0]

$Cl_3CCHFCl$

M 185.8
Liq. d_4^{20} 1.625 (1.619). Mp −95.4°. Bp 117°. n_D^{20} 1.4525 (1.4488).

Miller, W.T., *J. Am. Chem. Soc.*, 1940, **62**, 341 (*synth*)
Wilmshurst, J.K., *Can. J. Chem.*, 1957, **35**, 937 (*ir*)

IC-002981

C_2HCl_4F

1,1,2,2-Tetrachloro-1-fluoroethane, 9CI
Fluorocarbon 121
[354-14-3]

$Cl_2CFCHCl_2$

M 185.8
Liq. d_4^{20} 1.622. Mp −82.6°. Bp 115-117°. n_D^{20} 1.4487.

Miller, W.T., *J. Am. Chem. Soc.*, 1940, **62**, 341 (*synth*)
Alger, T.D. *et al*, *J. Chem. Phys.*, 1967, **47**, 3130 (*pmr, F-19 nmr*)
Paleta, O. *et al*, *Collect. Czech. Chem. Commun.*, 1968, **33**, 1294 (*synth*)

IC-002982

C_2HCl_5

Pentachloroethane, 9CI
Pentalin
[76-01-7]

Cl_2CHCCl_3

M 202.2
Obt. by chlorination of trichloroethene. Solvent and degreasing agent. Used in org. synth. Liq. with chloroform odour. d_4^{25} 1.671 (1.673). Fp −29°. Bp 162°, Bp_{37} 69°. n_D^{15} 1.5054.

▷ Highly toxic by inhalation and skin absorption. Mixt. with K is explosive. KI6300000.

Guyot, A., *Chim. Ind. (Paris)*, 1923, **10**, 13.
Timmermans, J. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1926, **23**, 747.
Tuaillon, J. *et al*, *Helv. Chim. Acta*, 1976, **59**, 171 (*synth*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 426.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2663.

IC-002983

C_2HF_3

Trifluoroethene, 9CI
Trifluoroethylene. Fluorocarbon 1123. 3FE
[359-11-5]

$F_2C{=}CHF$

M 82.0
Monomer for plastics. Gas. Fp −78°. Bp −61° to −60°, Bp_{628} −56°.

▷ Flammable.

Crosse, A.V. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 2289 (*synth*)
Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)
Craig, N.C. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 3047 (*synth*)
Tikhomirov, M.V. *et al*, *Zh. Fiz. Khim.*, 1967, **41**, 1065 (*ms*)
Galabov, B. *et al*, *J. Chem. Phys.*, 1979, **71**, 4716 (*ir*)
Bien, G. *et al*, *Chem. Phys.*, 1981, **60**, 61 (*pe, uv*)
Kushida, K. *et al*, *Proton and Fluorine Nuclear Magnetic Resonance Spectral Data*, Japan Halon Co Ltd, Japan,, 1988, 090, 091 (*F-19 nmr, pmr*)

IC-002984

C_2HF_4N

***N*-(Trifluoromethyl)fluoroformimide**
N-(Trifluoromethyl)fluoromethanimine, 11CI
[99298-36-9]

$F_3CN{=}CHF$

M 115.0
Formed as a mixt. of isomers, E:Z 6.7:1. Synth. from $F_3CN{\equiv}C$ + HF at 20°. Colourless gas. Bp 5°.

[99298-35-8]

Lentz, D. *et al*, *Inorg. Chem.*, 1985, **24**, 4665 (*synth, ir, ms, pmr, F-19 nmr, ed*)

IC-002985

C_2HF_5

Pentafluoroethane, 9CI
Fluorocarbon 125
[354-33-6]

F_3CCF_2H

M 120.0
Candidate refrigerant with low ozone depletion potential; non-flammable. Gas. Fp −103°. Bp −48.5°.

LaZerte, J.D. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 4525 (*synth*)
Elleman, D.D. *et al*, *J. Mol. Spectrosc.*, 1961, **7**, 307 (*nmr*)
Beagley, B. *et al*, *J. Mol. Struct.*, 1981, **71**, 203 (*struct*)
Compton, D.A.C. *et al*, *J. Phys. Chem.*, 1982, **86**, 1628 (*ir*)

IC-002986

C_2HF_5OS

Pentafluoro(2-oxoethenyl)sulfur
Pentafluoro-λ^6-sulfanylketene

$O{=}C{=}CHSF_5$

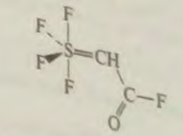
M 168.0
Formed from $F_5SCH_2CO_2H + P_4O_{10}$. Colourless liq., dimerises on heating. Bp 47°. Forms rubbery solid in presence of KF.
Dimer: $C_4H_2F_{10}O_2S_2$ M 336.1

Krügerke, T. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 799 (*synth, ir, ms, F-19 nmr*)

IC-002987

C_2HF_5OS

Tetrafluoro(2-fluoro-2-oxoethylidene)sulfur
Tetrafluoro-λ^6-sulfanylideneacetyl fluoride. Fluorocarbonylmethylidenesulfur tetrafluoride
[109907-09-7]



M 168.0
Interatomic distances: C=S 160.2, C—C 145.3, C=O 117.8, C—F 136.6 pm; angles: $F_{eq}SF_{eq}$ 101.72, $F_{ax}SF_{ax}$ 172.19, SCC 126.2, OCF 119°. Formed by thermal isomerisation of Pentafluoro(2-oxoethenyl)sulfur, IC-002986. Colourless liq. at r.t. Mp −29°.

Krügerke, T. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 799 (*synth, ir, pmr, F-19 nmr, ms, cryst struct*)

IC-002988

C_2HF_5S

(Ethynyl)pentafluorosulfur
Ethynylsulfur pentafluoride
[917-89-5]

$HC{\equiv}CSF_5$

M 152.0
Interatomic distances: F—S 157.4, S—C 172.7, C—C 120.2, C—H 106.4 pm. Formed from (2-Bromoethenyl) pentafluorosulfur, IC-002994 + KOH. Colourless gas. Bp 6°.

Hoover, F.W. *et al*, *J. Org. Chem.*, 1964, **29**, 3567 (*synth, ir, F-19 nmr*)
Canich, J.M. *et al*, *Inorg. Chem.*, 1985, **24**, 3668 (*synth, ir, F-19 nmr*)
Csaszar, A.G. *et al*, *Inorg. Chem.*, 1986, **26**, 955 (*synth, ed*)

IC-002989

$C_2HF_6NO_4S_2$

Bis[(trifluoromethyl)sulfonyl]imide
[82113-65-3]

$F_3CSO_2NHSO_2CF_3$

M 281.1
Synth. from $H_2NSO_2CF_3$ + NaOMe + $(Me_3Si)_2NH$ which yields $NaN(SO_2CF_3)_2$ followed by H_2SO_4. White cryst. fuming in moist air. Mp 49-50°.

N-Chloro: see N-*Chlorobis(trifluoromethylsulfonyl)imide, IC-002864*
N-Nitrosyl: [91742-19-7].
$C_2F_6N_2O_5S_2$ M 310.1
From corresp. N—Cl compd. + NO. Mp 118°.
Na salt: [91742-21-1].
$C_2F_6NNaO_4S_2$ M 303.1
White granular solid.
Cs salt: [91742-16-4].
$C_2CsF_6NO_4S_2$ M 413.0
Synth. from parent compd. + CsF in MeCN.

Foropoulos, J. *et al, Inorg. Chem.*, 1984, **23**, 3720 (*synth, ir, ms, F-19 nmr*)

$C_2HF_6NS_2$ IC-002990

Bis(trifluoromethane)sulfenimide
Bis(trifluoromethylmercapto)amine. 1,1,1-Trifluoro-N-[(trifluoromethyl)thio]methanesulfenamide, 9CI
[763-24-6]

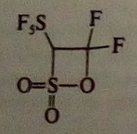
$(F_3CS)_2NH$

M 217.1
Synth. from CF_3SCl + NH_3. Colourless liq. Mp −47°. Bp 73° (extrap.).

Emeleus, H.J. *et al, J. Chem. Soc.*, 1960, 1103 (*synth, props, ir*)
Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1974, **406**, 185 (*reactions*)

$C_2HF_7O_3S_2$ IC-002991

(4,4-Difluoro-1,2-oxathietan-3-yl)pentafluorosulfur *S,S*-dioxide, 12CI
1-Pentafluoro-λ⁶-sulfanyl-2,2-difluoroethanesulfonic acid sulfone
[113591-65-4]



M 270.1
Synth. from $F_5SCH{=}CF_2$ and SO_3 at 100°. Stable cryst., hydrol. to $SF_5CH_2SO_2F$. Mp 47-48°. Bp_{600} 108-111°.

Terjeson, R.J. *et al, Inorg. Chem.*, 1988, **27**, 2916 (*synth, nmr, ir, ms, reactions*)

C_2HF_7S IC-002992

Tetrafluoro(2,2,2-trifluoroethylidene)sulfur
2,2,2-Trifluoroethylidenesulfur tetrafluoride
[88476-02-2]

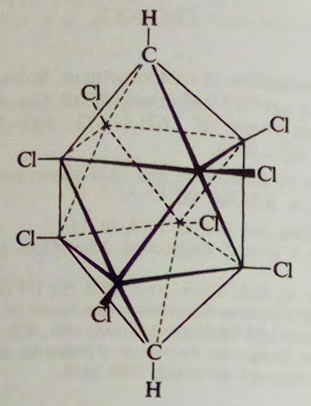
$F_3CCH{=}SF_4$

M 190.0
Synth. from $CF_3CH(Li)SF_5$ by LiF elimination. Stable colourless gas formed as a mixt. with $F_2C{=}CHSF_5$. Mp −98°. Bp 17°.

Poetter, B. *et al, Chem. Ber.*, 1984, **117**, 3255 (*synth, ir, ms, F-19 nmr*)
Poetter, B. *et al, J. Am. Chem. Soc.*, 1985, **107**, 980 (*reactions*)

$C_2H_2B_8Cl_8$ IC-002993

2,3,4,5,6,7,8,9-Octachloro-1,10-dicarbadecaborane(10), 9CI
[23642-17-3]



M 396.1
closo-. Colourless solid. Sol. CCl_4. Mp 179-180°.

Garrett, P.M. *et al, J. Am. Chem. Soc.*, 1969, **91**, 4707 (*synth, ir, pmr, B-11 nmr, ms*)

$C_2H_2BrF_5S$ IC-002994

(2-Bromoethenyl)pentafluorosulfur
2-Bromovinylsulfur pentafluoride. 1-Bromo-2-(pentafluorothio)ethene
[58636-82-1]

$BrCH{=}CHSF_5$

M 233.0
Formed from F_5SBr + $CH{\equiv}CH$ at 57°. Colourless liq. Bp 86°.

Canich, J.M. *et al, Inorg. Chem.*, 1985, **24**, 3668 (*synth, ir, F-19 nmr, ms*)

$C_2H_2CaO_4$ IC-002995

Calcium formate
Calcium methanoate. Formic acid, calcium salt, 8CI. Methanoic acid, calcium salt
[544-17-2]

$Ca(OOCH)_2$

M 130.1
Synth. from $CaCl_2$ + formic acid; or by reaction of CO with a calcium compd. ($Ca(OH)_2$, $CaCO_3$, CaS) in the presence of H_2O. Colourless orthorhombic cryst. Also exists in several other polymorphic forms. V. sol. H_2O (16.2 g per 100 cm^3 at 0°; 18.4 g per 100 cm^3 at 100°); insol. EtOH. Thermal dec. gives $CaCO_3$ via CaC_2O_4 with evolution of CO and H_2.

▷ LQ5600000.

Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 976 (*rev, bibl*)
Dollimore, D. *et al, Proc. Eur. Symp. Therm. Anal., 1st*, 1976, 233; *CA*, 1977, **87**, 125556 (*thermal dec*)
Burger, N. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 1968 (*cryst struct*)
Baraldi, P., *Spectrochim. Acta, Part A*, 1979, **35**, 1003 (*ir, thermal dec*)
Matsui, M. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 1081.
Matsui, M. *et al, Acta Crystallogr., Sect. A*, 1981, **37**, 728 (*polymorph*)

Fuess, H. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1981, **156**, 219 (*X-N density distribn*)
Miura, H. *et al, J. Chem. Phys.*, 1986, **85**, 2458 (*pmr*)
Terao, T. *et al, J. Chem. Phys.*, 1986, **85**, 3816 (*cmr*)

$C_2H_2CdO_4$ IC-002996

Cadmium formate
[4464-23-7]

$Cd(OOCH)_2$

M 202.4
In solid state Cd is 7-coord.; two different formates; (i) tridentate and (ii) quadridentate. Synth. from $CdCO_3$ and aq. HCOOH at *ca.* 77°. Catalyst for CO_2/ethylene oxide reaction. Colourless cryst. Sol. H_2O (~6.7 g per 100 cm^3 at 50°).
Dihydrate: [51006-62-3].
Synth. from CdO and aq. HCOOH. Cryst. Dehydrates in 2 stages at 67-83° and 90-112°. Struct. contains two different octahedral CdO_6 environments: Cd(1) ($4OH_2$ + 2 formate-*O*), Cd(2) (6 formate-*O*).

Haussühl, S., *Fortschr. Mineral.*, 1961, **39**, 332 (*cryst struct*)
Osaki, K. *et al, J. Phys. Soc. Jpn.*, 1963, **18**, 919 (*powder struct, dihydrate*)
Filipovic, I. *et al, Croat. Chim. Acta*, 1970, **42**, 541 (*stability const*)
Hoas, H. *et al, J. Chem. Phys.*, 1973, **58**, 3339 (*nqr*)
Post, M.L. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 1880 (*cryst struct, dihydrate*)
Itkina, L.S. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1244 (*ir, powder struct, salt and dihydrate*)
Baraldi, P., *Spectrochim. Acta, Part A*, 1979, **35**, 1003 (*ir, thermal dec, dihydrate*)
Weber, G., *Acta Crystallogr., Sect. B*, 1980, **36**, 1947 (*cryst struct*)
Post, H. *et al, J. Magn. Reson.*, 1980, **40**, 17 (*pmr*)
Mennitt, P.G. *et al, J. Phys. Chem.*, 1981, **85**, 2087 (*Cd-113 nmr, dihydrate*)
Nadzharyan, K.A. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 179 (*dihydrate*)
Chaplygina, N.M. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1985, **30**, 1238 (*synth, salt and dihydrate*)
Dec, S.F. *et al, J. Magn. Reson.*, 1986, **70**, 355 (*Cd-113 nmr*)
Gorski, A. *et al, J. Therm. Anal.*, 1987, **32**, 1243 (*thermal anal*)

C_2H_3ClF IC-002997

1-Chloro-1-fluoroethylene, 8CI
1-Chloro-1-fluoroethene, 9CI. Fluorocarbon 1131a
[2317-91-1]

$FCCl{=}CH_2$

M 80.4
Monomer for polymerisations. Gas. Mp −169°. Bp −24°.

U.S. Pat., 2 344 061, (1940); *CA*, **38**, 3297 (*manuf, synth*)
McConnel, H.M. *et al, J. Chem. Phys.*, 1956, **24**, 479 (*nmr*)

C_2H_3ClF IC-002998

1-Chloro-2-fluoroethylene
1-Chloro-2-fluoroethene, 9CI. Acetylene chlorofluoride. Fluorocarbon 1131
[460-16-2]

$ClHC{=}CHF$

M 80.4
(*E*)-*form* [2268-32-8]
Gas. Bp −4° to −3.5°.
(*Z*)-*form* [2268-31-7]
Gas or liq. Bp 15-15.5°.

Swarts, F., *Chem. Zentralbl.*, 1903, **1**, 13; *Bull. Soc. Chim. Fr.*, 1919, **25**, 153.
U.S. Pat., 2 377 297, (1945); *CA*, **39**, 4081.
Viehe, H.G. *et al, Chem. Ber.*, 1960, **93**, 1697 (*synth, nmr*)

$C_2H_2ClF_3$ IC-002999

1-Chloro-1,1,2-trifluoroethane
Fluorocarbon 133b
[421-04-5]

$ClCF_2CH_2F$

M 118.4
Working fluid for absorption refrigeration. Bp 12°.
[1330-45-6]

Haszeldine, R.N. *et al, J. Chem. Soc.*, 1957, 2800 (*synth*)
Dean, R.R. *et al, Trans. Faraday Soc.*, 1968, **64**, 1409 (*pmr, F-19 nmr*)

$C_2H_2ClF_3$ IC-003000

1-Chloro-1,2,2-trifluoroethane
Fluorocarbon 133
[431-07-2]

$F_2CHCHClF$

M 118.4
(±)-*form*
Aerosol propellant, working fluid for heat pumps. d_4^{10} 1.365. Bp 17° (20-23°).
[1330-45-6]

Haszeldine, R.N. *et al, J. Chem. Soc.*, 1960, 4503 (*synth*)
Rausch, D.A. *et al, J. Org. Chem.*, 1963, **28**, 494 (*synth*)
Horvath, A.L., *Chem. Eng.* (*N.Y.*), 1988, **95**, 155 (*props*)

$C_2H_2ClF_3$ IC-003001

2-Chloro-1,1,1-trifluoroethane
Fluorocarbon 133a
[75-88-7]

F_3CCH_2Cl

M 118.4
Metabolic by-product of halothane in rats. Shows anaesthetic props. Intermediate for manuf. of $CF_3CHClBr$ and CF_3CH_2F. d_4^0 1.389. Fp −105.5° (−101°). Bp 6.1°. n_D^0 1.309.

▷ Toxic, OES 5 ppm-fv/v.

[1330-45-6]

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1948, **70**, 1025 (*props*)
Rud Nielsen, J. *et al, J. Chem. Phys.*, 1953, **21**, 1060 (*ir, raman*)
Ellerman, D.D. *et al, J. Mol. Spectrosc.*, 1961, **7**, 307 (*pmr, F-19 nmr*)
Fuller, G. *et al, Tetrahedron*, 1962, **18**, 123 (*synth, ms*)
Hudlicky, M. *et al, Collect. Czech. Chem. Commun.*, 1965, **30**, 2491 (*synth*)
Green, R.G. *et al, J. Photochem.*, 1977, **6**, 375 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 3rd. Ed., 1978-1984, **10**, 861 (*props*)
Feiring, A.E., *J. Fluorine Chem.*, 1979, **14**, 7 (*synth*)
Ogata, T. *et al, J. Mol. Struct.*, 1986, **144**, 1 (*microwave, CS-33 spr*)

$C_2H_2ClF_7Te$ IC-003002

(2-Chloro-2,2-difluoroethyl)pentafluorotellurium
1-Chloro-1,1-difluoro-2-(pentafluorotellurio)ethane

$ClCF_2CH_2TeF_5$

M 322.0

Formed from $H_2C{=}CF_2 + F_2TeCl_2 + h\nu$. Colourless liq. Dec. slowly to TeF_4 at 25°

Grelbig, T. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **544**, 74 (*synth, F-19 nmr, pmr, ms*)

IC-003003

$C_2H_2Cl_2$

1,1-Dichloroethylene, 8CI

1,1-Dichloroethene, 9CI. Vinylidene chloride. R 1130a

[75-35-4]

$H_2C{=}CCl_2$

M 96.9

Manuf. by dehydrochlorination of 1,1,1-trichloroethane. Intermediate in production of plastics as comonomer with vinyl chloride, acrylonitrile, acrylates etc. Reacts with alcohols and halides to give carboxylic acids. Volatile liq. d^{20} 1.218. Fp −122.5°. Bp 31.7° (37°). n_D^{20} 1.4249. Readily polymerises.

▷ Mod. toxic by inhalation, OES 40 mg m^{-3} Exp. carcinogen. Extremely flammable. Rapidly absorbs O_2 forming violently explosive peroxide. Flash pt. −10°. KV9275000.

Kunichika, S. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1950, **53**, 407; *CA*, **47**, 5871 (*synth*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 118.

Miyajima, G. *et al*, *J. Phys. Chem.*, 1971, **75**, 331 (*cmr*)

Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91 (*haz*)

Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 279.

Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3476.

IC-003004

$C_2H_2Cl_2$

1,2-Dichloroethylene

1,2-Dichloroethene, 9CI. Acetylene dichloride. Dioform. R1130

[540-59-0]

ClHC=CHCl

M 96.9

Solvent, degreasant. Liq. with ethereal odour. Bp 55°. Gradually dec. by air and light.

▷ KV9360000.

(*E*)-*form* [156-60-5]

d_4^{15} 1.265. Mp −50°. Bp 48.4°, Bp_{745} 47°. n_D^{15} 1.4490. Slowly oxidises in air.

▷ Mod. toxic, OES 790 mg m^{-3}. Highly flammable, flash p. 2°. With strong alkalis forms spont. flammable HC≡CCl. KV9400000.

(*Z*)-*form* [156-59-2]

d_4^{15} 1.291. Mp −80°. Bp 60°. n_D^{25} 1.4435.

▷ KV9420000.

Chavanne, G., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1912, **154**, 776.

Ott, E., *Ber.*, 1942, **75**, 1517.

Truce, W.E. *et al*, *J. Org. Chem.*, 1962, **27**, 128.

McKean, D.C., *Spectrochim. Acta, Part A*, 1975, **31**, 1167 (*spectra*)

Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91 (*haz*)

Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 279.

Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1152.

IC-003005

$C_2H_2Cl_2F_2$

1,1-Dichloro-1,2-difluoroethane, 8CI

Fluorocarbon 132c

$FCCl_2CH_2F$

M 115.9

Component of photoresistant developers and removers. Bp 48.4°.

[25915-78-0]

Bissell, E.R. *et al*, *J. Org. Chem.*, 1964, **29**, 1591 (*synth, ir, F-19 nmr, pmr, props*)

IC-003006

$C_2H_2Cl_2F_2$

1,1-Dichloro-2,2-difluoroethane

Fluorocarbon 132a

[471-43-2]

$F_2CHCHCl_2$

M 134.9

Propellant for aerosols, photoresist. remover; cleaning solv. Component for CO_2 laser system. d_4^{17} 1.495. Bp 58-60°.

[25915-78-0]

Di Giacomo, A. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 1361 (*props*)
Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1960, 4503 (*synth*)
Gatowsky, H.S., *J. Chem. Phys.*, 1962, **36**, 3353 (*pmr, ir, F-19 nmr*)
Vold, R.L. *et al*, *J. Chem. Phys.*, 1972, **56**, 4787 (*pmr*)
Boguslavakaya, L.S. *et al*, *Zh. Org. Khim.*, 1982, **18**, 938 (*synth, F-19 nmr*)

IC-003007

$C_2H_2Cl_2F_2$

1,2-Dichloro-1,1-difluoroethane

Fluorocarbon 132b

[1649-08-7]

F_2CClCH_2Cl

M 134.9

Component of water-removing agents. Blowing agent, propellant, photoresist. remover. Working fluid for refrigerators and heat pumps; solvent. Shows anaesthetic props. d_4^{20} 1.416. Fp −101°. Bp 45-47°. n_D^{20} 1.362.

▷ KI0950000.

[25915-78-0]

Smart, B.E., *Kirk-Othmer Encycl. Chem. Technol.*, **10**, 861 (*props*)
Deviney, M.L. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 4915 (*props*)
Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1957, 2193 (*synth*)
Bucket, H.P. *et al*, *J. Mol. Spectrosc.*, 1963, **11**, 47 (*ir, raman*)
Dean, R.R. *et al*, *Trans. Faraday Soc.*, 1968, **64**, 1409 (*F-19 nmr*)
Green, R.G. *et al*, *J. Photochem.*, 1977, **6**, 375 (*uv*)
Feiring, A.E., *J. Fluorine Chem.*, 1979, **14**, 7 (*synth*)

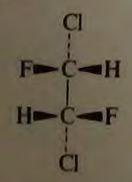
IC-003008

$C_2H_2Cl_2F_2$

1,2-Dichloro-1,2-difluoroethane

Fluorocarbon 132

[431-06-1]



(*1RS,2RS*)-*form*

M 134.9

Photoresist remover; solvent; shows anaesthetic props.

(*1RS, 2RS*)-*form* [33489-30-4]

(±)-*form*

d_4^{20} 1.4744. Fp −155°. Bp 59.4°. n_D^{20} 1.3790.

(*1RS, 2SR*)-*form* [33579-37-2]

meso-*form*

Bp 59.9°.

[25915-78-0]

Haszeldine, R.N., *J. Chem. Soc.*, 1952, 4259 (*synth*)
Rausch, D.A. *et al*, *J. Org. Chem.*, 1963, **28**, 494 (*synth*)
Bissell, E.R. *et al*, *J. Org. Chem.*, 1964, **29**, 1591 (*synth, pmr, F-19 nmr, props*)
Stewart, J.R. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 6017 (*F-19 nmr*)
Laszlo, V. *et al*, *J. Chromatogr.*, 1971, **62**, 458 (*chromatog*)
Abraham, R.J. *et al*, *Org. Magn. Reson.*, 1974, **6**, 331 (*F-19 nmr*)
Boguslavskaya, L.S. *et al*, *Zh. Org. Khim.*, 1982, **18**, 938 (*synth, pmr*)

IC-003009

$C_2H_2Cl_2F_2O_2S$

Bis(chlorofluoromethyl) sulfone

Sulfonylbis(chlorofluoromethane), 12CI

$(HClFC)_2SO_2$

M 199.0

Formed as mixt. of isomers, separated by gc. Synth. by hydrol. of 2,4-dichloro-2,4-difluoro-1,3-dithietane-1,1,3-trioxide. Colourless liq. Bp_6 67° (mixt.).

(*RS, RS*)-*form* [108319-79-5]

(±)-*form*

Characterised spectroscopically. Solid. Mp 32-34°.

(*RS, SR*)-*form* [108319-90-0]

meso-*form*

Characterised spectroscopically. Solid. Mp 32-34°.

Henn, R. *et al*, *Chem. Ber.*, 1987, **120**, 1499 (*synth, ir, ms, F-19 nmr, pmr, cmr*)

IC-003010

$C_2H_2Cl_3F$

1,1,1-Trichloro-2-fluoroethane

Fluorocarbon 131b

[2366-36-1]

Cl_3CCH_2F

M 151.3

Propellent for aerosols. Component of resin foams. Bp 86-87°. n_D^{20} 1.4250.

[27154-33-2]

Luft, N.W., *J. Phys. Chem.*, 1955, **59**, 92 (*props*)
Boguslavskaya, L.S. *et al*, *Zh. Org. Khim.*, 1982, **18**, 2082 (*synth, pmr*)

IC-003011

$C_2H_2Cl_3F$

1,1,2-Trichloro-1-fluoroethane

Fluorocarbon 131a

[811-95-0]

Cl_2CFCH_2Cl

M 151.3

Prepd. by reaction of HF with trichloroethene using BF_3 catalyst. Component of aerosols. Solvent for extraction of essential oils and for cleaning. d_4^{20} 1.492. Fp −104.7°. Bp 85.5-86°. n_D^{20} 1.4270.

[27154-33-2]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 404 (*synth, props*)
Boguslavskaya, I.S. *et al*, *J. Fluorine Chem.*, 1978, **12**, 257 (*synth, pmr*)

IC-003012

$C_2H_2Cl_3F$

1,1,2-Trichloro-2-fluoroethane

Fluorocarbon 131

[359-28-4]

$Cl_2CHCClF$

M 151.3

(±)-*form*

Lead scavenger in motor fuel. d_4^{20} 1.538. Bp 102.5°.

Bp_{752} 101°. n_D^{20} 1.4390.

[27154-33-2]

Hermon, M., *Ind. Chim. Belg.*, 1951, **16**, 86 (*raman*)
Di Giacomo, A. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 1361 (*props*)
Gutowsky, H.S. *et al*, *J. Chem. Phys.*, 1962, **36**, 3353 (*pmr, F-19 nmr*)
Martynov, I.V. *et al*, *Zh. Obshch. Khim.*, 1965, **35**, 967 (*synth*)
Dean, R.R. *et al*, *Trans. Faraday Soc.*, 1968, **64**, 1409 (*F-19 nmr*)
Gambaretto, G.P. *et al*, *J. Fluorine Chem.*, 1976, **7**, 569 (*synth, ir, pmr*)

IC-003013

$C_2H_2Cl_4$

1,1,1,2-Tetrachloroethane, 9CI

asym-*Tetrachloroethane*

[630-20-6]

Cl_3CCH_2Cl

M 167.8

Manuf. by partial chlorination of acetylene. Solvent, metal degreasing agent, component of paint removers, varnishes, lacquers. Oil and fat extractant. Used in org. synth. Intermediate for manuf. of other chlorinated hydrocarbons. Liq. d_0^{25} 1.542. Fp −68.1°. Bp 135.1° (130.5°).

▷ An experimental carcinogen; skin and eye irritant; evolves toxic fumes on dec., KI8450000.

Kokatnur, V.R., *J. Am. Chem. Soc.*, 1919, **41**, 123 (*synth*)
Prins, H.J., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1926, **45**, 80.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3189.

IC-003014

$C_2H_2Cl_4$

1,1,2,2-Tetrachloroethane, 9CI

sym-*Tetrachloroethane. Acetylene tetrachloride*

[79-34-5]

$Cl_2CHCHCl_2$

M 167.8

Nonflammable solv. for fats, resins, etc. Liq. with chloroform-like odour. d_4^{25} 1.59. Fp −43.8°, Mp −36° (−44°). Bp 146.3°, Bp_{45} 62°.

▷ Highly toxic by ingestion, inhalation (OES 1 ppm v/v) and skin contact. KI8575000.

Timmermans, J., *Bull. Soc. Chim. Belg.*, 1927, **36**, 502.
Favorskii, A.E. *et al*, *CA*, 1935, **29**, 7271 (*synth*)
Field, K. *et al*, *J. Org. Chem.*, 1971, **36**, 3566 (*synth*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 496.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3189.

IC-003015

$C_2H_2Cl_4N_2Ti$

Tetrachlorobis(hydrogen cyanide)titanium(*IV*)

Tetrachlorobis(hydrocyanic acid)titanium(IV), 9CI. *Tetrachlorobis(formonitrile)titanium*(IV). *Titanium*(IV) *chloride bis(hydrogen cyanide)*

$(HC{\equiv}N)_2TiCl_4$

M 243.7

cis-form [34750-81-7]
Synth. from $TiCl_4$ and HCN in a sealed tube. A temperature gradient 80-20° yields cryst. at the cold end. Yellow cryst. solid. Rapidly dec. in air. Sol. liq. HCN. Ir ν_{CN} 2135 cm^{-1}.

▷ Hydrol. releasing HCN.

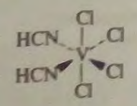
[27757-43-7]

Constant, G. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1969, **269**, 975 (*synth, ir*)
Constant, G. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 2388 (*cryst struct, ir*)
Choplin, F. *et al*, *Theor. Chim. Acta*, 1972, **25**, 54 (*theory*)

$C_2H_2Cl_4N_2V$ IC-003016

Tetrachlorobis(hydrocyanic acid)vanadium(*IV*), 9CI
Tetrachlorobis(formonitrile)vanadium(IV). *Vanadium*(IV) *chloride bis(hydrogen cyanide)*

[30752-88-6]



M 246.8
Octahedral.

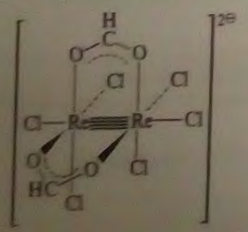
▷ Highly toxic: HCN is evolved on heating.

cis-form [42221-78-3]
Synth. from HCN (g.) with VCl_4 (liq.) in a sealed tube from 80°→25°. Black air-sensitive cryst. Dec. > 40° releasing HCN.

Constant, G. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **271**, 361 (*synth, ir, us-cis*)
Constant, G. *et al*, *J. Coord. Chem.*, 1973, **2**, 303 (*cryst struct*)

$C_2H_2Cl_6O_4Re_2^{2\ominus}$ IC-003017

Hexachlorobis[μ-(formato-*O*:*O*′)]dirhenate(*III*)(2 –), 9CI



M 675.1 (ion)
Interatomic distances: Re—Cl_{ax} 217, Re—Cl_{eq} 231, Re—Re 226.0pm.

Di-NH_4 salt: [52375-56-1].
Monoclinic dark blue, glistening cryst. or dark green cryst. solid. Sol. HCO_2H; spar. sol. Me_2CO, EtOH. Diamagnetic. In aq. soln., at r.t., blue soln. v. slowly turns green and a dark brown hydrolysis product appears.

[12540-25-9, 61177-62-6, 61177-63-7, 95543-28-7]

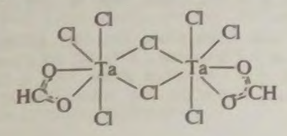
Kotel'nikova, A.S. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1969, **10**, 1012 (*synth*)
Kuz'min, P.A. *et al*, *Zh. Strukt. Khim.*, 1974, **15**, 64; *J. Struct. Chem. USSR (Engl. Transl.)*, 1974, **15**, 56 (*synth, cryst struct*)
Kuz'min, P.A. *et al*, *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 1484 (*props*)

Osmanov, N.S. *et al*, *Zh. Neorg. Khim.*, 1988, **33**, 628; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1988, **33**, 353 (*improved synth, props, ir, raman*)

$C_2H_2Cl_8O_4Ta_2$ IC-003018

Di-μ-chlorohexachlorobis(formato-*O*,*O*′)ditantalum(*V*), 11Cl
Tantalum(V) *tetrachloride formate dimer*

[88430-25-5]



M 735.5
Struct. is based on ir evidence only. Synth. by adding 1 mol. HCOOH to 1 mol. $TaCl_5$ in C_6H_6.

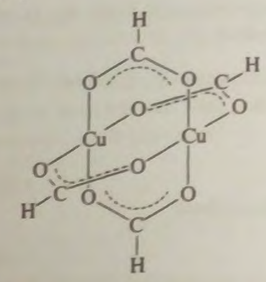
Monomer:
$CHCl_4O_2Ta$ M 367.7

Viard, B. *et al*, *J. Chem. Res. (S)*, 1983, 252 (*synth, ir*)

$C_2H_2CuO_4$ IC-003019

Copper(*II*) formate
Cupric formate. Tubercuprose

[544-19-4]



dimer

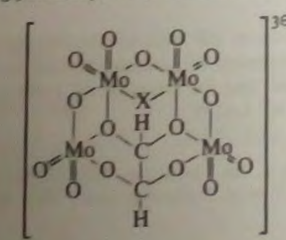
M 153.5
Anhydrous form is dimeric. Dihydrate and tetrahydrate also exist. Antibacterial agent in cellulose treatment.

Tetrakis*[*μ*-(*formato-O:O′*)]*dicopper*, *11Cl [67551-60-4]
$C_4H_4Cu_2O_8$ M 307.1
Three forms exist: powder blue, turquoise or royal blue cryst. Sol. H_2O, insol. org. solvs.

Martin, R.L. *et al*, *J. Chem. Soc.*, 1959, 1359 (*synth, magnetism, props*)
Hoffmann, S. *et al*, *J. Magn. Reson.*, 1986, **68**, 490 (*esr*)
Merck Index, 11th Ed., 1989, No. 2642.

$C_2H_2FMo_4O_{15}^{3\ominus}$ IC-003020

μ_4-[1,1,2,2-Ethanetetrolato(4 –)-*O*^{1}:*O*^{1},*O*^{2}:*O*$^{1\prime}$:*O*$^{1\prime}$,*O*$^{2\prime}$]-μ-fluorotri-μ-oxooctaoxotetramolybdate(3 –), 10Cl
μ-Fluoro-μ-glyoxalatopenta-μ-oxooctaoxotetramolybdate



X = F

M 668.7 (ion)
Interatomic distances: Mo—Mo 460.3, 327.1, 329.4; Mo—F 222.4, 365.1, 312.9 pm.

Tris-tetrabutylammonium salt: [74791-98-3].
Block-shaped cryst. + $1CH_2Cl_2$ (CH_2Cl_2/toluene).

Day, V.W. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 5971 (*cryst struct*)

$C_2H_2FNaO_2$ IC-003021

Sodium fluoroacetate
Fluoroacetic acid, sodium salt, 8CI. 2-Fluoroethanoic acid, sodium salt

[62-74-8]

$NaOOCCH_2F$

M 100.0
Synth. by careful neutralisation of Na_2CO_3 with aq. FCH_2COOH. Manuf. by fluorination of $CH_2ClCONH_2$ with SbF_3 followed by treatment with NaOH. Commercially available. Rodenticide. White powder; monoclinic cryst. V. sol. H_2O (111 g per 100 cm^3 at 25°); spar. sol. EtOH (1.4 g per 100 cm^3 at 25°); prac. insol. Me_2CO (0.04 g per 100 cm^3 at 25°); CCl_4 (0.0049 g per 100 cm^3 at 25°). Mp 200°.

▷ Highly toxic, corrosive. AH9100000.

Phillips, M.A., *Ind. Chem.*, 1954, **30**, 122 (*manuf*)
Spinner, E., *J. Chem. Soc.*, 1964, 4217 (*ir, raman*)
Wade, D.A., *A.S.T.M. Spec. Tech. Publ.*, STP635 Test Methods Vertebr. Pest Control Manage. Mater., Symp., 1977, 157 (*rev, predacide*)
Vedavathi, B.M. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 946 (*cryst struct*)
Egekeze, J.O. *et al*, *Vet. Hum. Toxicol.*, 1979, **21**, 411 (*rev, tox*)
Kang, I. *et al*, *Aust. J. Chem.*, 1986, **39**, 465 (*ir*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1691C (*haz*)

$C_2H_3F_3$ IC-003022

1,1-Difluoroethylene
1,1-Difluoroethene, 9CI. Vinylidene fluoride. Fluorocarbon 1132a. VDF

[75-38-7]

$H_2C{=}CF_2$

M 64.0
Obt. by hydrogenation of $CF_2{=}CCl_2$. Odourless gas. Fp −144°. Bp −83°.

▷ Flammable, toxic by inhalation. KW0560000.

Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1957, 2800 (*synth*)
Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961 (*rev*)
Madai, H. *et al*, *J. Prakt. Chem.*, 1963, **19**, 202 (*synth*)
Curion, J.L. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1974, **70**, 177 (*struct*)
Mijlhoff, F.C. *et al*, *J. Mol. Struct.*, 1977, **39**, 241 (*struct*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 292.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3476.

$C_2H_3F_3$ IC-003023

1,2-Difluoroethylene
1,2-Difluoroethene

[1691-13-0]

FCH=CHF

M 64.0

(*E*)-*form* [1630-78-0]
Bp −53.1°.
(*Z*)-*form* [1630-77-9]
Gas. Bp −26.0°.
Haszeldine, R.N. *et al*, *J. Chem. Soc.*, 1957, 2800 (*synth*)
Craig, N.C. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 3047 (*synth, ir, props*)
Coyle, T.D. *et al*, *J. Chem. Soc.*, 1961, 743 (*pmr, F-19 nmr*)
Flynn, G.W. *et al*, *J. Chem. Phys.*, 1963, 2295 (*synth, nmr*)

$C_2H_3F_4$ IC-003024

1,1,2,2-Tetrafluoroethane, 9CI
Fluorocarbon 134. HFC 134

[359-35-3]

F_2CHCHF_2

M 102.0
Gas. Fp −89°. Bp −19.7°.

▷ Flammable.

[29759-38-4]

Young, D.S. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 1171 (*synth*)
Knunyants, I.L. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1958, 906 (*synth*)
Dean, R.R. *et al*, *Trans. Faraday Soc.*, 1968, **64**, 1409 (*pmr, F nmr*)

$C_2H_2FeO_4$ IC-003025

Iron(*II*) formate
Iron(II) *methanoate. Bis(formato)iron*(II)

$Fe(HCOO)_2$

M 145.8
Obt. as dihydrate.

Dihydrate:
$C_2H_6FeO_6$ M 181.9
Pale green platelets (EtOH aq.); cryst. form depends on solv. ratio during crystallisation. Sol. H_2O; insol. EtOH. Loses H_2O at 140-145°; dec. ⩾ 200°.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1930, **B3**, 518 (*rev, bibl*)
Inorg. Synth., 1953, **4**, 159 (*synth*)

$C_2H_2HgO_6$ IC-003026

Mercury(*II*) hydrogen carbonate ($Hg(HCO_3)_2$)
Mercury(II) *bicarbonate*

$Hg(HCO_3)_2$

M 322.6
Precipitated at 0° from $KHCO_3$ + $Hg^{2\oplus}$. Stable at r.t. under a CO_2 atm.

Grover, K.C., *J. Indian Chem. Soc.*, 1948, **25**, 489 (*synth*)
Grover, K.C., *Agra Univ. J. Res.*, 1957, **6**, 67; *C.A.* **53**, 6855c (*synth*)

$C_2H_2Hg_2O_4$ IC-003027

Bis(formato)dimercury
Mercury(I) *formate dimer*

[5930-36-9]

HCOOHgHgOOCH

M 491.2
From $Hg_2(NO_3)_2$ and NaOOCH in dil. aq. acid at −10°. If prepared at r.t., some dec. is indicated by grey colouration. Used as electrode. Light sensitive solid + $2H_2O$ (H_2O). Sol. warm H_2O; insol. cold H_2O. Readily dec. on warming to Hg, HCOOH and CO_2.

Muller, G.A. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 1871 (*synth, stability*)
Haas, P., *Nature (London)*, 1951, **167**, 325.
Chauchard, J. *et al*, *Bull. Soc. Chim. Fr.*, 1966, 2635 (*use*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B**, 1264 (*rev, bibl*)
Ostannii, N.I. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1974, **48**, 209 (*use*)

$C_2H_2INaO_2$ IC-003028

Sodium iodoacetate

Sodium iodoethanoate. Iodoacetic acid, sodium salt, 8CI. 2-Iodoethanoic acid, sodium salt

[305-53-3]

$NaOOCCH_2I$

M 207.9

Synth. by neutralisation of Na_2CO_3 with aq. CH_2ICOOH. Commercially available. White powder. Sol. H_2O. Mp 208° dec.

▷ Toxic; irritant; induces osteoarthrosis. AI3675000.

Spinner, E., *J. Chem. Soc.*, 1964, 4217 (*ir, raman*)
Kalbhen, D.A., *Int. Congr. Ser.-Excerpta Med.*, (Degener. Jt.), 1985, **668**, 299; *CA*, 1986, **104**, 66752 (*tox*)
Kang, I. *et al*, *Aust. J. Chem.*, 1986, **39**, 465 (*ir*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1992C (*haz*)

$C_2H_2MnO_4$ IC-003029

Manganese(*II*) formate

[3251-96-5]

$Mn(OOCH)_2$

M 144.9

Synth. from the dihydrate at 100-120°. Forms $[Mn(OOCH)_4]^{2\ominus}$ with formate. Sol. H_2O. $\mu_{eff} = 5.71\mu_B$. Rehydrates in moist air, struct. contains octahedral Mn(*II*).

Dihydrate: [4247-36-3]. *Diaquabis(formato-O)manganese*(II)
$C_2H_6MnO_6$ M 181.0
Synth. from $MnCO_3$ and formic acid. Red cryst. (HCOOH aq.). Struct. contains MnO_6 and *trans*-$MnO_2(OH_2)_4$ octahedra. Canted antiferromagnetic arrangement below T_N. $T_N \simeq 3.7$K.

Osaki, K. *et al*, *J. Phys. Soc. Jpn.*, 1964, **19**, 717 (*cryst struct*)
Eckhardt, R.C. *et al*, *Trans. Faraday Soc.*, 1964, **60**, 1289 (*synth*)
Dollimore, D. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 621 (*synth*)
Kay, M.I. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 1312 (*cryst struct, dihydrate*)
Thomas, J.M. *et al*, *J. Chem. Soc. A*, 1970, 2938 (*struct*)
Burlet, P. *et al*, *Phys. Status Solidi B*, 1975, **71**, 675 (*magnetism*)
Ogata, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 1674 (*ir*)
Arkhangel'skii, I.V. *et al*, *Sov. J. Coord. Chem. (Engl. Transl.)*, 1977, **3**, 292 (*struct*)
Rao, J.L., *Solid State Commun.*, 1978, **28**, 243 (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 1 (*rev, bibl*)
Weber, G., *Z. Kristallogr.*, 1982, **158**, 315 (*cryst struct, dihydrate*)

$C_2H_2N_2$ IC-003030

Ethenediimine

Dicarbodiimide

[20815-45-6]

$HN{=}C{=}C{=}NH$

M 54.0

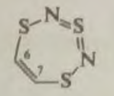
Formed by low pressure pyrolysis of cyanimide with matrix isoln.

King, S.T. *et al*, *J. Chem. Phys.*, 1971, **54**, 1289 (*synth, ir*)

$C_2H_2N_2S_3$ IC-003031

1,3,5,2,4-Trithia(3-5^{IV})diazepine, 9CI

[90350-43-9]



M 150.2

Volatile cryst. Mp 57°.

6,7-Dihydro: [97484-09-8].
$C_2H_4N_2S_3$ M 152.2
Synth. from $Me_3SiN{=}S{=}NSiMe_3$ + $ClSCH_2CH_2SCl$. Orange solid. Mp 30°. $Bp_{0.3}$ 45°.

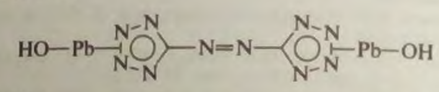
Jones, R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 398 (*cryst struct*)
Morris, J.L. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1987, 211, 217 (*synth, uv, ir, pmr, cmr, ms, props*)

$C_2H_2N_{10}O_2Pb_2$ IC-003032

[μ-[[5,5′-Azobis[1*H*-tetrazolato]](2−)]]dihydroxydilead, 9CI

Basic lead azotetrazole. Bis[hydroxolead(II)*] 5,5′-azotetrazolediide*

[94015-57-3]



M 612.5

Prepd. by mixing aq. solns. of $Pb(OAc)_4$ and di-Na azotetrazolide at 90° in the presence of NH_4OH. Suitable for explosive priming. Yellow cryst. Ignition temp. 222° when heated at a 5° increase per min.

▷ Explosive.

U.K. Pat., 986 631, (1965); *CA*, **62**, 16260b (*synth*)
Whelan, D.J. *et al*, *Thermochim. Acta*, 1984, **80**, 149 (*thermal dec*)

$C_2H_2O_4Pb$ IC-003033

Lead(*II*) formate

Formic acid lead(2+) salt, 9CI

[811-54-1]

$Pb(OOCH)_2$

M 297.2

Has a 3-D polymeric struct. Cryst. Mp 190° dec.

Harvey, K.B. *et al*, *Can. J. Chem.*, 1963, **41**, 1181 (*ir*)
Donaldson, J.D. *et al*, *Spectrochim. Acta*, 1964, **20**, 847 (*ir*)
Harrison, P.G. *et al*, *J. Organomet. Chem.*, 1982, **239**, 105 (*cryst struct*)

$C_2H_2O_4Sn$ IC-003034

Tin(*II*) formate

Bis(formato)tin. Formic acid, tin(2+) salt, 9CI. Bis(formyloxy)tin

[2879-85-8]

$Sn(OOCH)_2$

M 208.7

Synth. from HCOOH and SnO. White cryst. Dec. without melting at 198-200°.

Donaldson, J.D. *et al*, *J. Chem. Soc.*, 1964, 4801 (*synth*)
Donaldson, J.D. *et al*, *Spectrochim. Acta*, 1964, **20**, 847 (*ir*)
Donaldson, J.D. *et al*, *J. Chem. Soc. A*, 1968, 1448 (*mössbauer*)
Harrison, P.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1274 (*cryst struct, ir, mössbauer*)

$C_2H_2O_4Te$ IC-003035

Tellurodicarbonic acid, 9CI

$Te(COOH)_2$

M 217.6

Di-Et ester: [125106-61-8].
$C_6H_{10}O_4Te$ M 273.7
Liq. with characteristic odour. Bp_1 89°. Dec. on attempted chemical manipulation.

Suzuki, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1989, **62**, 2117 (*synth*)

$C_2H_2O_4Zn$ IC-003036

Zinc formate

[557-41-5]

$Zn(OOCH)_2$

M 155.4

Phenol-formaldehyde resin, trans-esterification and cross-linking catalyst. Used in paper coatings; pressure sensitive copying paper; wood preservative and in blowing agents. Cryst. Dec. to ZnO at >350°.

▷ LR0550000.

Dihydrate: [5970-62-7].
Cryst. Dehydrates at 85-120°. Isomorphous with Mg, Sr, Cd and Mn analogues.

Semenenko, K.N., *Zh. Neorg. Khim.*, 1957, **2**, 2115 (*synth, dihydrate*)
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1963-1971, **22**, 604.
Filipov, I. *et al*, *Croat. Chim. Acta*, 1970, **42**, 541 (*stability const*)
Burger, N. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1975, **145**, 346 (*cryst struct, dihydrate*)
Baraldi, P., *Spectrochim. Acta, Part A*, 1979, **35**, 1003 (*ir, salt and dihydrate*)
Mu, J. *et al*, *Thermochim. Acta*, 1981, **49**, 207 (*thermal anal, salt and dihydrate*)
Tewari, G.D. *et al*, *Appl. Spectrosc.*, 1982, **36**, 441 (*ir, raman, salt and dihydrate*)
Grigor'ev, A.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 497 (*ir*)
Gorski, A. *et al*, *J. Therm. Anal.*, 1987, **32**, 1243 (*thermal anal*)

$C_2H_2O_8Pb_3$ IC-003037

Lead carbonate hydroxide

Basic lead(II) *carbonate. White lead. Bis[carbonato(2−)] dihydroxytrilead, 9CI. C.I. Pigment White 1*

[1319-46-6]

$2PbCO_3.Pb(OH)_2$

M 775.6

Prepd. by treating $Pb(OAc)_2$ with CO_2. Was the most important white pigment used in paints but has now been largely replaced by TiO_2. Cryst. Insol. H_2O, EtOH. Mp 400° dec.

▷ Toxic.

Mineral-form [1319-47-7]
Hydrocerussite
Occurs as a secondary mineral in oxidised ore. Grey, white to colourless trigonal cryst.

Lemke, A. *et al*, *Z. Anorg. Allg. Chem.*, 1934, **220**, 312 (*synth*)
Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1951, **2**, 270 (*mineral*)
Olby, J.K., *J. Inorg. Nucl. Chem.*, 1966, **28**, 2507 (*cryst struct*)
Andreeva, V.N. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 2089; *CA*, **73**, 115181c (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1981, **14**, 171 (*rev*)
Brooker, M.H. *et al*, *Can. J. Chem.*, 1983, **61**, 494 (*ir, raman*)

$C_2H_2S_6Te$ IC-003038

Tellurium bis(trithiocarbonic acid)

Bis(carbonotrithioato-S)tellurium

$HSC(S){-}S{-}Te{-}S{-}C(S)SH$

M 346.0

Isol. as ester.

S,S-Di-Et ester: [95786-94-0]. *Tellurium bis(ethyltrithiocarbonate)*
$C_6H_{10}S_6Te$ M 402.1
Orange needles. Sol. CH_2Cl_2. Mp 51-52°.

Karo, S. *et al*, *Z. Naturforsch., B*, 1985, **40**, 273 (*synth, ir, uv, pmr, reactions*)

$C_2H_3AgO_2$ IC-003039

Silver(*I*) acetate (AgOAc)

[563-63-3]

AgOAc

M 166.9

Dimeric.

▷ AJ4100000.

Dimer: [55906-24-6]. *Bis[μ-(acetato-O:O′)]disilver*
$C_4H_6Ag_2O_4$ M 333.8
Oxidising agent for use in liq. ammonia. White to greyish lustrous needles or crystalline powder. Light sensitive. Spar. sol. cold H_2O. Sol. dil. nitric acid. ΔH_f° −392.3 kJ mol^{-1}.

Matthews, F.W. *et al*, *Anal. Chem.*, 1950, **22**, 514 (*powder struct*)
Bonner, W.A. *et al*, *J. Chem. Educ.*, 1962, **39**, 639 (*ir*)
Yakerson, V.I. *et al*, *Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1963, 1003; *CA*, **59**, 123956 (*thermodyn*)
Pascual, C. *et al*, *Helv. Chim. Acta*, 1966, **49**, 1344 (*ir*)
Kline, R.J. *et al*, *Inorg. Chem.*, 1966, **5**, 932 (*synth, use*)
Adams, S.K. *et al*, *Inorg. Chim. Acta*, 1975, **12**, 163 (*ms, ir*)
Merck Index, 11th Ed., 1989, No. 8451.

$C_2H_3AlCl_4O$ IC-003040

(Acetyl chloride)trichloroaluminium

[26273-09-6]

$[H_3CCO][AlCl_4]$

M 211.8

Contrast struct. of Trichloro(propanoyl chloride) aluminium, IC-003616. From H_3CCOCl and $AlCl_3$. May be intermed. in Friedel Crafts reaction. White v. hygroscopic cryst. ($SOCl_2/CHCl_3$ 1:1).

le Carpentier, J.-M. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 1421 (*synth, cryst struct*)

$C_2H_3AlO_5$ IC-003041

Aluminium formate hydroxide ($Al(OOCH)_2OH$)

Aluminium hydroxide bis(formate). Monobasic aluminium formate. Bis(formato-O)hydroxyaluminium

[51575-25-8]

$Al(OH)(OOCH)_2$

M 134.0
Synth. from hydrated alumina + HCOOH or from $Al_2(SO_4)_3$, and CaO. Marketed as aq. soln. Mordant and antiperspirant. Used in waterproofing and increasing soil resistance of textiles, paper. Binder for glass fibre insulation. White solid (H_2O).

Toubes, B., *Kirk-Othmer Encycl. Chem. Technol.*, 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 202.

C_2H_3AuClN IC-003042

Chloro(isocyanomethane)gold
Chloro(methyl isocyanide)gold
[37131-30-9]

ClAuCNMe

M 273.4
Useful starting material for synth. of carbene complexes. Cryst. (CH_2Cl_2 or Me_2CO). Sol. CH_2Cl_2, Me_2CO. Mp 211° (from CH_2Cl_2), Mp 224° (from acetone).

Bonati, F. *et al*, *Gazz. Chim. Ital.*, 1973, **103**, 373 (*synth*)
Browning, J. *et al*, *J. Chem. Res. (S)*, 1978, 328; *J. Chem. Res. (M)*, 4201 (*nmr, ir*)

$C_2H_3AuCl_3N$ IC-003043

(Acetonitrile)trichlorogold, 9CI
Trichloro(acetonitrile)gold
[53747-67-4]

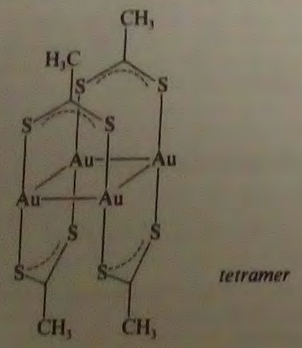
$Cl_3AuNCCH_3$

M 344.3
Orange-yellow cryst. (MeCN).

Kharasch, M.S. *et al*, *J. Am. Chem. Soc.*, 1934, **56**, 2057 (*synth, rev*)
Belli Dell'Amico, D. *et al*, *Gazz. Chim. Ital.*, 1973, **103**, 1099 (*synth, nmr*)

$C_2H_3AuS_2$ IC-003044

(Dithioacetato)gold(*I*)
Gold(I) *dithioacetate. (Ethanedithioato)gold*



tetramer

M 288.1
Tetrameric.
Tetramer: [74165-53-0]. *Tetrakis[μ-(ethanedithioato-S:S')] tetragold, 10CI*
$C_8H_{12}Au_4S_8$ M 1152.5
Air-stable cryst. (CS_2). Mean Au—Au distance 301 pm.

Piovesana, O. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1980, **19**, 561 (*synth, cryst struct*)

$C_2H_3Br_4NORe^{\ominus}$ IC-003045

(Acetonitrile)tetrabromooxorhenate(*V*)(1−)

$[O{=}ReBr_4(NCCH_3)]^{\ominus}$ (C_{4v})

M 562.8 (ion)
Octahedral. Acetonitrile complex of Tetrabromorhenate(*V*) (1−), IC-002051.

trans-form
Interatomic distances: Re=O 173, Re—N 231, Re—Cl (mean) 248 pm.

Ph_4As salt: Synth. by recryst. of Ph_4As [$ReOBr_4$] from MeCN. Red cryst. (MeCN).

Cotton, F.A. *et al*, *Inorg. Chem.*, 1966, **5**, 9, 416 (*synth, props, cryst struct*)

$C_2H_3Br_5NOs^{\ominus}$ IC-003046

(Acetonitrile)pentabromoosmate(*IV*)(1−)
Pentabromo(ethanenitrile)osmate(IV)
[63985-25-1]

$[OsBr_5(NCCH_3)]^{\ominus}$

M 630.7 (ion)
Presumed octahedral.
K salt: [63984-67-8].
Synth. by irradiation of a soln. of $K_2[OsBr_6]$ in MeCN.
Et_4N salt: [86365-52-8].
Synth. from $[Et_4N]_2[OsBr_4]$ and PbO_2 in MeCN at r.t.
Tetrabutylammonium salt: [63985-26-2].
Synth. by irradiation of a soln. of $[Bu_4N]_2[OsBr_6]$ in MeCN.

Hasenpusch, W. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **432**, 107 (*synth*)
Magnuson, R.H., *Inorg. Chem.*, 1984, **23**, 387 (*synth, uv*)

C_2H_3Cl IC-003047

Vinyl chloride
Chloroethene, 9CI. Chloroethylene. R 1140
[75-01-4]

$H_2C{=}CHCl$

M 62.4
Manuf. by thermal dehydrochlorination of 1,2-dichloroethane or by reaction of acetylene with HCl over mercury-based catalysts. Refrigerant. Polymerised by light or catalysis to PVC, an industrial polymer with numerous uses. Gas at r.t. d_4^{20} 0.912. Fp −159.7°. Bp −13.9°. n_D^{20} 1.4046.

▷ Human carcinogen, OES 7 ppm-fv/v (max. exp. limit), irritant. Highly flammable, flash p. −78°, may form unstable polyperoxide. KU9625000.

Dana, L.I. *et al*, *J. Am. Chem. Soc.*, 1927, **49**, 2801 (*synth*)
U.S. Pat., 1 926 638, (1933); *CA*, **27**, 5756 (*synth*)
U.S. Pat., 1 934 324, (1934); *CA*, **28**, 488 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3nd Ed., Wiley, N.Y., 1978-1984, **23**, 865 (*rev, props, bibl, use*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91 (*haz*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 530.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3473.

$C_2H_3ClF_2$ IC-003048

1-Chloro-1,1-difluoroethane, 9CI
Fluorocarbon 1426
[75-68-3]

H_3CCF_2Cl

M 100.4
Obt. by chlorination of 1,1-difluoroethane under u.v. irradiation or by reaction of 1,1,1-trichloroethane with HF. Refrigerant, solvent, chemical intermed. Gas. Fp −130.8°. Bp −9.5°.

▷ Low toxicity, flammable. KH7650000.

Brown, J.H. *et al*, *CA*, 1949, **43**, 2924 (*synth*)
Ger. Pat., 2 137 806, (1972); *CA*, **76**, 99093 (*synth*)
Barlos, K. *et al*, *Chem. Ber.*, 1978, **111**, 1833 (*nmr*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 802.

$C_2H_3ClF_2$ IC-003049

1-Chloro-1,2-difluoroethane
Fluorocarbon 142a
[338-64-7]

FCH_2CHClF

M 100.4
(±)-*form*
Bp 35°. n_D^{20} 1.3416.
[25497-29-4]

Rausch, D.A. *et al*, *J. Org. Chem.*, 1963, **28**, 494 (*synth*)

$C_2H_3ClF_2$ IC-003050

2-Chloro-1,1-difluoroethane
Fluorocarbon 142
[338-65-8]

F_2CHCH_2Cl

M 100.4
Used in the manuf. of 2,2-Difluoroethanol. Halothane metabolite showing anaesthetic props. d_4^{15} 1.312. Bp 35.1° (36°). n_D^{15} 1.3528.
[25497-29-4]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 889 (*synth*)
Robbins, B.H., *J. Pharmacol.*, 1946, **86**, 197 (*pharmacol*)

$C_2H_3ClO_3Ti$ IC-003051

(Acetato-*O*)chlorooxotitanium(*IV*)
Titanium(IV) *acetate chloride oxide*
[87687-05-6]

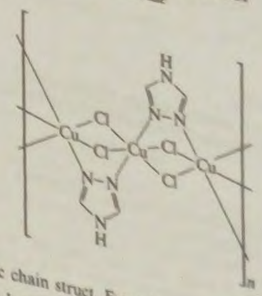
TiClO(OAc)

M 158.3
Synth. by hydrol. of $Cp_2TiClOAc$.

Knizhnikov, V.A. *et al*, *Vesti. Akad. Navuk. BSSR, Ser. Khim. Navuk.*, 1983, 102; *CA*, **99**, 195144z (*synth*)

$C_2H_3Cl_3CuN_3$ IC-003052

Dichloro(1*H*-1,2,4-triazole-*N*⁴)copper, 11Cl
1,2,4-Triazolecopper(II) *dichloride*
[26893-82-3]



M 203.5
Polymeric chain struct. Emerald green cryst.

Jarvis, J.A.J. *et al*, *Acta Crystallogr.*, 1960, **13**, 1027 (*cryst struct*)
Inoue, M. *et al*, *Inorg. Chem.*, 1965, **4**, 626; 1966, **5**, 70 (*synth, magnetism, pmr*)
Lavrenova, L.G. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 442 (*synth, ir, uv, magnetism, thermal props*)
Subramanian, S. *et al*, *Phys. Rev. B: Condens. Matter*, 1984, **30**, 3709 (*esr, uv*)
Ogleznova, S.M. *et al*, *Zh. Neorg. Khim.*, 1984, **29**, 1476 (*ir*)

$C_2H_3Cl_2F$ IC-003053

1,1-Dichloro-1-fluoroethane, 9CI
1-Fluoro-1,1-dichloroethane. HCFC 141B
[1717-00-6]

H_3CCCl_2F

M 116.9
Alternative refrigerant to Fluorocarbon 11 in foam blowing applications. d_4^{10} 1.250. Fp −103.5°. Bp 32°. n_D^{25} 1.360.

▷ Shows anaesthetic props.

Brown, J.H. *et al*, *J. Soc. Chem. Ind., London*, 1948, **67**, 331 (*synth*)
Smith, D.C. *et al*, *J. Chem. Phys.*, 1952, **20**, 473 (*ir, raman*)
Durig, J.R. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 175 (*ir, raman*)

$C_2H_3Cl_2F$ IC-003054

1,1-Dichloro-2-fluoroethane
F141a
[430-53-5]

Cl_2CHCH_2F

M 116.9
Liq. Bp 73-75° (est.).

Woolf, A.A., *J. Fluorine Chem.*, 1990, **50**, 89.

$C_2H_3Cl_2F$ IC-003055

1,2-Dichloro-1-fluoroethane, 9CI
Fluorocarbon 141
[430-57-9]

$ClCH_2CHFCl$

M 116.9
(±)-*form*
Prepd. by reaction of 1,1,2-trichloroethane with HgF_2. Cleaning solvent. Blowing agent for polyisocyanate resins. d_4^{20} 1.381. Bp 75.7°. n_D^{20} 1.4113.

[25167-88-8]

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 889 (*synth*)
El Bermani, M.F. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 1251 (*ir, raman*)
Gambarotto, G.P. *et al*, *J. Fluorine Chem.*, 1976, **7**, 569 (*synth, pmr*)

IC-003056

$C_2H_3Cl_2GaO_2$

Gallium(*III*) acetate chloride (Ga(OAc)Cl$_2$)

Acetato(dichloro)gallium. Gallium(III) *dichloride ethanoate*

$GaCl_2(OAc)$

M 199.6
Synth. from Gallium(*III*) acetate, IC-005047 + HCl or $GaCl_3$. Colourless moisture sensitive cryst. Sol. H_2O, alcohols. Spar. sol. Et_2O.

Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **330**, 70 (*synth*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 1105.

IC-003057

$C_2H_3Cl_2O_3Ta$

(Acetato-*O*)dichlorooxotantalum(*V*), 11Cl

[86677-00-1]

$TaO(OAc)Cl_2$

M 326.8
Chain struct. with Ta—O—Ta links. Synth. from $TaCl_5$ and Ac_2O or AcOH. The resulting mixture of (Acetato-*O*)tetrachlorotantalum(*V*), IC-003069 and $TaO(OAc)Cl_2$ is separated in C_6H_6 soln. Yellow solid.

Viard, B. *et al*, *J. Chem. Res. (S)*, 1983, 84 (*synth, ir*)

IC-003058

$C_2H_3Cl_3$

1,1,1-Trichloroethane, 9Cl, 8Cl

Methylchloroform. α-Trichloroethane

[71-55-6]

Cl_3CCH_3

M 133.4
Used in wide range of industrial cleaning and degreasing operations. Nonflammable liq. Insol. H_2O. d_4^{20} 1.34. Mp −32.5°. Bp 74.1°.

▷ Mod. toxic, OES 1900 mg m^{-3}. Vapour can ignite or explode if heated. Reacts with Al. Production controlled by environmental legislation. KJ2975000.

Sutton, L.E., *Proc. R. Soc. London, A*, 1931, **133**, 673 (*synth*)
U.S. Pat., 2 209 000, (1940); *CA*, **35**, 140 (*synth*)
Riddick, J.A. *et al*, *Organic Solvents*, Wiley-Interscience, 3rd Ed., 1970, 777 (*purifn, props*)
Bretherick, L., *Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91 (*haz*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 513.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3327.

IC-003059

$C_2H_3Cl_3$

1,1,2-Trichloroethane, 9Cl, 8Cl

β-Trichloroethane

[79-00-5]

$ClCH_2CHCl_2$

M 133.4
Industrial solv. Nonflammable, mobile liq. with pleasant odour. Insol. H_2O, misc. most org. solvs. d_4^{20} 1.442. Mp −35.5° (−36.7°). Bp 113-114°, $Bp_{75.9}$ 49.97°.

▷ Mod. toxic, OES 45 mg m^{-3} (under review). KJ3150000.

Prins, H.J., *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1926, **45**, 80 (*synth*)
Netherlands Pat., 6 414 743, (1965); *CA*, **64**, 590 (*manuf*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 514.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3328.

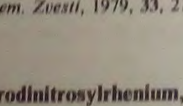
IC-003060

$C_2H_3Cl_3NOV$

(Acetonitrile)trichlorooxovanadium(*V*), 9Cl

Oxotrichloro(methyl cyanide)vanadium(V)

[56390-05-7]



M 214.3
Square based pyramid with vanadium 39 pm above the basal plane. Synth. by dissolving $VOCl_3$ in MeCN, purif. by subl. Subl. 30° *in vacuo*.

[33516-03-9]

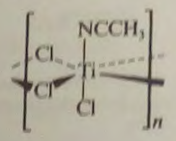
Brunette, J.P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci, Sect. C*, 1971, **272**, 2147 (*synth, ir, uv-vis*)
Daran, J.C. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1833 (*cryst struct*)

IC-003061

$C_2H_3Cl_3NTi$

(Acetonitrile)trichlorotitanium(*III*), 10Cl

Titanium(III) *chloride acetonitrile*



M 195.2
It is not clear that the reported monomer and polymer are different. Magnetic data suggest a polymeric struct. Tentative struct. shown. Synth. by thermal dec. of $TiCl_3.3MeCN$.

Monomeric-form [15614-91-2]
Brown air-sensitive solid. Paramagnetic, $\mu_{eff} = 1.37\mu_B$, g = 1.911 (297K); $\mu_{eff} = 1.09\mu_B$, g = 1.907 (77K).

Polymeric-form [36658-61-4]
Green solid. Paramagnetic, $\mu_{eff} = 1.37\mu_B$ (300K).

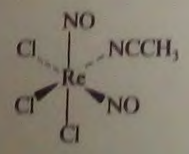
Fowles, G.W.A. *et al*, *J. Chem. Soc. A*, 1967, 517 (*synth, uv-vis*)
Hoff, G.R. *et al*, *Inorg. Chem.*, 1971, **10**, 2063 (*synth, ir, uv-vis, magnetism, esr*)
Zikmund, M. *et al*, *Chem. Zvesti*, 1979, **33**, 217 (*synth*)

IC-003062

$C_2H_3Cl_3N_3O_2Re$

(Acetonitrile)trichlorodinitrosylrhenium, 11Cl

[80529-32-4]



M 393.6
Synth. from $Re(NO)_2Cl_3$ and MeCN. Green cryst. (*MeCN*).

Mronga, N. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **482**, 95 (*synth, ir, cryst struct, props*)

IC-003063

$C_2H_3Cl_3O_2Ti$

(Acetato-*O*)trichlorotitanium(*IV*), 11Cl, 9Cl

Titanium acetate trichloride

[5908-59-8]

$TiCl_3OAc$

M 213.2
Synth. from $TiCl_4$ + 1 mol. HOAc at r.t. Has been used to catalyse the polym. of α-olefins. Yellow solid. Forms $Ti(OAc)_2Cl_2$ with excess HOAc but further substitution is not obsd. Both are v. moisture-sensitive. Insol. CCl_4, pet. ether.

NOCl complex: [19126-60-4].
$C_2H_3Cl_4NO_3Ti$ M 278.7
Synth. by condensing NOCl at 0° onto parent compd.

Bis-Py complex: [104881-52-9]. (*Acetato*-O)*trichlorobis(pyridine)titanium*(IV), *11Cl*
$C_{12}H_{13}Cl_3N_2O_2Ti$ M 371.4
Synth. from parent compd. + Py. Yellow solid.

[37960-29-5, 39019-81-3]

Amaudrut, J. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 2228; 1975, 1933 (*synth, ir*)
Mach, K. *et al*, *Collect. Czech. Chem. Commun.*, 1975, **40**, 326 (*ir, pmr, reaction*)
Belg. Pat., 884,739, (1977); *CA*, **95**, 8060b (*use*)
Viard, B. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1089 (*props, deriv*)
Kapoor, R. *et al*, *Indian J. Chem., Sect. A*, 1986, **25**, 271 (*synth, Py deriv*)

IC-003064

$C_2H_3Cl_4GaO$

(Acetyl chloride)trichlorogallium

Acetyl tetrachlorogallate. 1-Oxoethylium tetrachlorogallate(1−). Acetyl chloride - gallium trichloride

[36608-31-8]

$[H_3CCO][GaCl_4]$

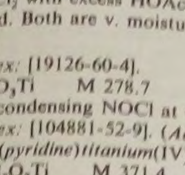
M 254.5
Synth. from MeCOCl and $GaCl_3$. White v. hygroscopic cryst. ($SOCl_2/CHCl_3$ 1:1). Corresp. $[EtCO]^{\oplus}$ compd. also descr.

Le Carpentier, J.-M. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 1421, 1430 (*synth, cryst struct*)

IC-003065

$C_2H_3Cl_4MoNO^{\ominus}$

(Acetonitrile)tetrachlorooxomolybdate(*V*)(1−), 11Cl, 10Cl



M 294.8 (ion)
Distorted octahedral struct.

$[AsPh_4]_2[MoOCl_4]$ *salt:* [73495-78-0].
Dark green cryst. Sol. MeCN, CH_2Cl_2.

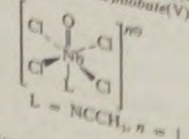
Weller, F. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **460**, 191 (*cryst struct, synth, ir*)

IC-003066

$C_2H_3Cl_4NNbO^{\ominus}$

(Acetonitrile)tetrachlorooxoniobate(*V*)(1−), 11Cl

Oxotetrachloro(methyl cyanide)niobate(V)(1−)



M 291.7 (ion)
$MePh_3P$ salt: [87692-98-6]
Synth. from $NbCl_5$ and CCl_3NO_2 to form $NO[NbOCl_4]$ followed by addition of $MePh_3PCl$ and MeCN.

Dehnicke, K. *et al*, *Chem.-Ztg.*, 1983, **107**, 247 (*synth*)
Hiller, W. *et al*, *Z. Naturforsch., B*, 1984, **39**, 107 (*cryst struct*)

IC-003067

$C_2H_3Cl_4NTi$

(Acetonitrile)tetrachlorotitanium(*IV*), 11Cl

Titanium(IV) *chloride acetonitrile*

[13682-81-0]

$(H_3CCN)TiCl_4$

M 230.7
Synth. either by direct reaction between $TiCl_4$ and MeCN or by oxidising Ti with Cl_2 in MeCN soln.

Hathaway, B.J. *et al*, *J. Chem. Soc.*, 1965, 537 (*synth, ir, uv-vis*)
Perkins, P.G. *et al*, *J. Chem. Soc. A*, 1970, 3229 (*synth, thermochem*)
Kuz'min, A.I. *et al*, *Koord. Khim.*, 1982, **8**, 159; *CA*, **96**, 154238c (*Cl-35 nqr*)

IC-003068

$C_2H_3Cl_4N_2ORe$

(Acetonitrile)tetrachloronitrosylrhenium(*IV*), 9Cl

[52620-60-7]

$Re(NO)Cl_4(NCCH_3)$

M 399.0
cis-Octahedral. Synth. from $ReCl_5$ and NO in CCl_4 followed by treatment with MeCN. Dark brown powder or green cryst. (MeCN).

[55516-59-1]

Buslaev, Yu.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 402 (*synth, ir, props*)
Khodashova, T.S. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 409 (*synth, ir, cryst struct*)

IC-003069

$C_2H_3Cl_4O_2Ta$

(Acetato-*O*)tetrachlorotantalum(*V*), 11Cl

[86676-99-5]

$TaCl_4(OAc)$

M 381.8
Yellow solid.

Dimer: Bis(acetato-O,O′)di-μ-chlorohexachloroditantalum(V), *11Cl*
$C_4H_6Cl_8O_4Ta_2$ M 763.6
Synth. from $TaCl_5$ + HOAc (1:1) in C_6H_6. Dimeric in C_6H_6; struct. based on spectroscopic evidence. Analogous compds. known for other carboxylates, eg. formate, butanoate, trifluoroacetate.

Viard, B. *et al*, *J. Chem. Res. (S)*, 1983, 84, 252 (*synth, ir*)

IC-003070

$C_2H_2Cl_3NTa$

(Acetonitrile)pentachlorotantalum(V), 1ICl

Tantalum(V) chloride acetonitrile

[12012-49-6]

$MeCNTaCl_5$

M 399.2

Synth. by recryst. of $TaCl_5$ from MeCN. White cryst.

Fowles, R. *et al. J. Chem. Soc.*, 1964, 2042 (*synth*)
Werbach, A. *et al. Bull. Chim. Acta*, 1971, **54**, 2543 (*pmr*)
Ray, A.R. *et al. J. Less-Common Met.*, 1978, **61**, 1 (*thermochem, ab-init*)
Burstein, B.E. *et al. Inorg. Chem.*, 1986, **25**, 851 (*electrochem*)

IC-003071

$C_2H_2Cr_3O_{10}$

Acetatodi-μ-oxotetraoxotrichromium

$Cr_3(OAc)O_8$

M 359.0

Formed as a graphite intercalate.

Graphite intercalate: [100984-91-0]

Synth. by reaction of CrO_3 and graphite in acetic acid soln. Solid. Unit cell contains a $(CrO_3)_3$ trimer and an acetic acid, which links trimers to form zig-zag chain.

Kobayashi, T. *et al. J. Phys. Chem.*, 1986, **90**, 2253 (*cryst struct*)

IC-003072

$C_2H_3CsO_2$

Caesium acetate

Acetic acid, caesium salt, 8CI. Ethanoic acid, caesium salt

[3396-11-0]

CsOAc

M 191.9

Prepd. by slow neutralisation of Cs_2CO_3 with AcOH in aq. soln. Commercially available. Widely used in catalysis. Deliquescent, white hexagonal cryst. V. sol. H_2O (945 g per 100 cm^3 at 2.5°; 1346 g per 100 cm^3 at 89°). Mp 194°.

Gmelin Handbook Inorg. Chem., Syst. No. 25, 1955, 240 (*rev, bibl*)
Hashizume, J. *et al. Acta Crystallogr., Sect. B*, 1972, **28**, 3099 (*cryst struct*)
Nadtrov, E.G., *CA*, 1978, **89**, 120881 (*pr*)
Sigma-Aldrich Library of Chemical Safety Data 1988, **2**, 715A.

IC-003073

$C_2H_3CuO_2$

Copper(I) acetate

Cuprous acetate, 1Acetato-O,O'copper, 8CI

[13978-05-1]

$[CuOAc]_n$

M 122.5

Polymeric planar chains in solid state. Transparent leafy cryst. Dec. on heating. Rapidly hydrol. by H_2O.

[598-54-9]

Auger, A. *et al. J. Chem. Soc.*, 1902, 1385 (*synth*)
Shimizu, H. *et al. J. Am. Chem. Soc.*, 1952, **74**, 4469 (*synth*)
Lin, D.C.K. *et al. Can. J. Chem.*, 1972, **50**, 2999 (*rec*)
Ogura, T. *et al. Inorg. Chem.*, 1975, **12**, 2611 (*rec*)
Drew, M.G.B. *et al. J. Chem. Soc., Chem. Commun.*, 1975, 124 (*synth, cryst struct*)
Luckhurst, T.P. *et al. Polyhedron*, 1985, **4**, 1745 (*synth*)
Merck Index, 11th Ed., 1989, 2665.

IC-003074

C_2H_3F

Fluoroethylene

Fluoroethene. Vinyl fluoride. Fluorocarbon 1141

[75-02-5]

$H_2C{=}CHF$

M 46.0

Odourless gas. Insol. H_2O, sol. EtOH, Me_2CO. Fp −160.5°. Bp −51° (−72°, −66°). Burns with a green flame, polymerises easily to poly(vinyl fluoride).

▷ Forms explosive mixts. with air. Toxic by inhalation. YZT3510000.

Swarts, F., *Bull. Soc. Chim. Fr.*, 1919, **25**, 193 (*synth*)
Newkirk, A.E., *J. Am. Chem. Soc.*, 1946, **68**, 2467 (*synth*)
Cohen, F.S., *Encycl. Polym. Sci. Technol.*, 1971, **14**, 522 (*rev*)
Hudlicky, M., *Chemistry of Organic Fluorine Compounds*, 2nd Ed., Wiley, London, 1976, 803.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 531.
Sax, N.I. *et al. Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3476.

IC-003075

$C_2H_3F_3$

1,1,1-Trifluoroethane

Methylfluoroform. Fluorocarbon 143a

[420-46-2]

F_3CCH_3

M 84.0

Anaesthetic. Gas. d_4^{20} 1.176. Mp −111.3°. Bp −47° to −46°.

▷ Flammable.

Henne, A.L. *et al. J. Am. Chem. Soc.*, 1936, **58**, 889 (*synth*)
McBee, E.T. *et al. Ind. Eng. Chem.*, 1947, **39**, 419 (*props, synth*)
Whalley, W.B., *J. Soc. Chem. Ind., London*, 1947, **66**, 427 (*synth*)
Thompson, H.W. *et al. J. Chem. Soc.*, 1948, 1428 (*ir*)
Mottier, F.L. *et al. J. Chem. Phys.*, 1954, **22**, 394 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **10**, 857; **11**, 65.
Buerger, H. *et al. Spectrochim. Acta, Part A*, 1980, **36**, 7 (*ir, raman, pmr*)
Eujen, R. *et al. J. Fluorine Chem.*, 1983, **22**, 263 (*F-19 nmr*)

IC-003076

$C_2H_3F_3$

1,1,2-Trifluoroethane

Fluorocarbon 143

[430-66-0]

F_2CHCH_2F

M 84.0

Refrigerant, aerosol propellant. Solvent used in the manuf. of electronic components. Component of photocopier inks. Fp −84°. Bp 5° (3°).

[27987-06-0]

Hasseldine, R.N. *et al. J. Chem. Soc.*, 1960, 4503 (*synth*)
Mukhtarov, I.A., *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1963, 151, 1076.
Abraham, R.J. *et al. J. Chem. Soc. B*, 1971, 1240 (*pmr, F-19 nmr*)
Beagley, B. *et al. J. Mol. Struct.*, 1979, **54**, 175 (*ed, props*)
Kalinnsky, V.F. *et al. J. Phys. Chem.*, 1982, **86**, 1351 (*ir, raman*)

IC-003077

$C_2H_3F_4NO_2S$

(Cyanato-*N*)tetrafluoro(methanolato)sulfur

Tetrafluoromethoxy-λ⁶-sulfanyl isocyanate

$O{=}C{=}NS(OMe)F_4$

M 181.1

Stereochem. not specified. Synth. from F_3SNCO + Me_3SiOMe. Colourless liq. Mp −130° (glass). Bp 56°.

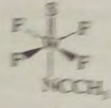
Thrasher, J.S. *et al. J. Am. Chem. Soc.*, 1986, **108**, 3524 (*synth, ir, pmr, F-19 nmr, ms*)

IC-003078

$C_2H_4F_4NSW$

Acetonitriletetrafluorothioxotungsten(VI), 1ICl, 1MCl, 9Cl

[59082-10-3]



M 332.9

trans-Octahedral. Synth. from WF_5 + H_2S in MeCN. Light yellow-green cryst. Rapid hydrol. in air → H_2S. Readily sol. MeCN; spar. sol. CH_2Cl_2. Mp 146° dec.

[65108-53-0, 88586-71-4]

Kuhlmann, Yu.V. *et al. Koord. Khim.*, 1976, **2**, 766; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1976, **2**, 605 (*synth, F-19 nmr, ir*)
Holloway, J.H. *et al. J. Chem. Soc., Chem. Commun.*, 1985, 1079.

IC-003079

C_2H_4KOS

Potassium thioacetate

Ethanethioic acid, potassium salt, 9Cl. Thioacetic acid, potassium salt, 8Cl. Thiethanoic acid, potassium salt. Potassium thioethanoate

[10387-40-3]

$K[OC(S)CH_3]$

M 114.2

Obt. by neutralisation of thioacetic acid, using K_2CO_3 or KOH. Commercially available. Reagent for synth. of thiols from halides. Moisture-sensitive orthorhombic cryst.

Hopkins, R.L. *et al. CA*, 1964, **60**, 13185e (*synth*)
Reid, M.M. *et al. Acta Crystallogr., Sect. B*, 1974, **30**, 2777.
Bernard, M.A. *et al. Ber. Chim. Minér.*, 1975, **12**, 181 (*ir*)
Farina, S. *et al. Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1978, **287**, 581 (*uses*)
Kato, S. *et al. Z. Naturforsch., B*, 1983, **38**, 1585 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2911B (*loc*)

IC-003080

$C_2H_4KO_2$

Potassium acetate

Acetic acid, potassium salt, 8CI. Ethanoic acid, potassium salt

[127-08-2]

KOAc

M 98.1

Synth. by neutralisation of aq. HOAc with KOH or K_2CO_3. Commercially available. Catalyst, esp. for polym., esterification and gasification processes. White monoclinic powder; deliquescent. Converts to a second monoclinic modification at 76° and undergoes a monoclinic to orthorhombic transition at 140°. Dec. on heating forming $K_2C_2O_4$ as intermed. and K_2CO_3 as final prod. V. sol. H_2O (253 g per 100 cm^3 at 20°; 492 g per 100 cm^3 at 62°), MeOH (24 g per 100 cm^3 at 15°), EtOH; insol. Et_2O, Me_2CO. Mp 292°. ΔH_f° −725 kJ mol^{-1}.

▷ 42012000.

Gregor, et, J.-L., *Zh. Neorg. Khim.*, 1961, **6**, 902 (*ir*)
Peters, R.A. *et al. Analyst (London)*, 1971, **96**, 720 (*pmr*)
Hoffmann, J. *et al. Acta Crystallogr., Sect. B*, 1971, **28**, 3100 (*struct, polymorph*)
Bear, S.G. *et al. Can. J. Chem.*, 1972, **50**, 3924 (*E-O mmr*)
Bertolo, P., *Spectrochim. Acta, Part A*, 1987, **38**, 21 (*ir, thermal dec*)
Jeffrey, J.E. *et al. J. Phys. Chem. Solids*, 1985, **46**, 345 (*polymorphs, raman*)
Hoffmann, K. *et al. Mikrochim. Chim.*, 1986, **III**, 9 (*pmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 715C (*loc*)

IC-003081

$C_2H_4Li_2O_3$

Lithium acetate

Acetic acid, lithium salt, 8Cl. Ethanoic acid, lithium salt

[546-89-4]

$LiOAc$

M 65.9

Prepd. by slow neutralisation of Li_2CO_3 with HOAc in aq. soln., crystn. as the dihydrate. Dec. on heating with formation of Li_2O. Mp 286°.

Dihydrate [6108-17-4]. Efflorescent

$C_2H_4Li_2O_3 \cdot 2H_2O$ M 102.9

Commercially available. White orthorhombic cryst. Dec. on heating to H_2O (max. 9 wt. H_2O [300 g per 100 cm³ at 15°], 9 wt. EtOH).

Andrianidisagara, T. *et al. Acta Crystallogr.*, 1958, **11**, 896 (*cryst struct, dihydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1960, 107 (*rec, diff, dihydrate*)
Kitaev, I.N. *et al. J. Chem. Soc. Spec. Publ.*, 1967, **19**, 147 (*cryst struct*)
Caldeira, M., *J. Mol. Spectrosc.*, 1968, **2**, 193 (*ir, cryst struct, dihydrate*)
Merck Index, 11th Ed., 1989, No. 5506.

IC-003082

$C_2H_5MnN_2O_3$

(Isocyanato)(trimethylphosphine)

(Methyl isocyanato)trimethylphosphine

[83962-23-0]

$MeN(CMe_3)NO_3$

M 186.1

Synth. from $Na[Mn(NO)_3(CN)]$ and $[Me_3O]BF_4$ at 20° in MeCN. Deep-red microcryst. (pentane). Mp 27°. Ir: ν_{NO} 2205cm; ν_{MO} 1790s, 1702vs cm^{-1} (hexane).

Moll, M. *et al. Z. Naturforsch., B*, 1983, **38**, 431 (*synth, ir, mm, mr*)

IC-003083

$C_2H_5Mn_2O_{10}^{3\ominus}$

μ_4-[1,1,2,2-Ethanetetrolato(4−)-$\kappa O^1:O^1:O^2:O^2$:$\kappa O^1:O^1:O^2:O^2$]bis[hydroxy(μ-oxo)manganate(3−)]

[μ-[2]Hydroxyacetaldehydato(2−)-$\kappa O^1:O^2$]hydroxy(μ-oxo)manganate(3−), *p*-Glyoxalato-*p*-hydroxy(μ-oxo)manganate(3−)

As μ_4-[1,1,2,2-Ethanetetrolato(4−)-$\kappa O^1:O^1:O^2:O^2$:$\kappa O^1:O^1:O^2:O^2$]fluoro(μ-oxo)manganate(3−), IC-003020 with

X = OH

M 666.7 (*ion*)

Tetranuclear anion. Interatomic distances: Mn—Mn 514.3, 323.1, 367.5 pm.

Tris-tetrabutylammonium salt: [74594-39-1]

Cryst. + CH_2Cl_2 (CH_2Cl_2/toluene).

Day, V.W. *et al. J. Am. Chem. Soc.*, 1980, **102**, 5971 (*cryst struct, synth, pmr*)

C_2H_3N IC-003084

Ethenimine, 9CI

Vinylideneamine. Keteneimine

[17619-22-6]

$H_2C{=}C{=}NH$

M 41.0

Transient species, rapidly tautomerizes to acetonitrile. Obs. at 14K and 77K.

Jacox, M.E., *Chem. Phys.*, 1979, **43**, 157 (*synth, ir, uv*)
Guillemin, J.-C. *et al, J. Chem. Soc., Chem. Commun.*, 1983, 238 (*synth, ir*)
Rodler, M. *et al, Chem. Phys. Lett.*, 1984, **110**, 447 (*synth, bibl*)
Wentrup, C. *et al, J. Am. Chem. Soc.*, 1988, **110**, 1337 (*props, bibl*)

$C_2H_3NS_3$ IC-003085

***N*-(Thioformyl)dithiocarbamic acid**

N-(Thioformyl)carbamodithioic acid

HC(S)NHC(S)SH

M 137.2

Isol. as Me ester.

Me ester: [102118-24-1]. *Methyl* N-(*thioformyl*) *dithiocarbamate*

$C_3H_5NS_3$ M 151.2

Synth. from $S_2CNHC(S)H^{\ominus}$ + MeI in Et_2O. Orange cryst., polym. on standing. Sol. $CHCl_3$. Mp 104-105°.

Gerner, R. *et al, Z. Anorg. Allg. Chem.*, 1985, **525**, 112 (*synth, ir, ms, pmr, cmr*)

$C_2H_3NaO_2$ IC-003086

Sodium acetate

Acetic acid, sodium salt, 8CI. Ethanoic acid, sodium salt

[127-09-3]

NaOAc

M 82.0

Synth. by reaction of NaOH with EtOH at 250-280° or by treatment of EtOAc with metallic Na or $NaNH_2$. Commercially available. Food additive, polym. catalyst. White powder. V. sol. H_2O (119 g per 100 cm^3 at 0°; 170 g per 100 cm^3 at 100°); spar. sol. EtOH. Mp 324°. ΔH_f° −710 kJ mol^{-1}.

▷ AJ4375000.

Trihydrate: [6131-90-4].

$C_2H_9NaO_5$ M 136.0

Cryst. from aq. soln. of NaOAc. Commercially available. Used in heat storage systems. Colourless monoclinic cryst., efflorescent. Dec. on heating by H_2O loss (−$3H_2O$ at 123°). V. sol. H_2O (76 g per 100 cm^3 at 0°; 139 g per 100 cm^3 at 50°); sol. EtOH (2.1 g per 100 cm^3 at 18°), Et_2O. ΔH_f° −1605 kJ mol^{-1}.

Rossini, F.D. *et al, Natl. Bur. Std. Circ. (U.S.)*, No. 500, 1952, 470 (*thermochem props*)
Padmanabhan, V.M., *Proc. - Indian Natl. Sci. Acad., Part A*, 1953, **37**, 401 (*trihydrate, raman*)
Jones, L.H. *et al, J. Chem. Phys.*, 1954, **22**, 1796 (*trihydrate, ir*)
Flett, M., *Spectrochim. Acta*, 1962, **18**, 1537 (*ir*)
Spinner, E., *J. Chem. Soc.*, 1964, 4217 (*raman*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1024 (*uses*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1412, 1418 (*rev, bibl*)
Kirichenko, E.A., *Zh. Strukt. Khim.*, 1976, **17**, 379 (*struct*)
Wei, K.T. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 522 (*trihydrate, struct*)
Aue, W.P. *et al, J. Chem. Phys.*, 1984, **80**, 1729 (*cmr*)

Tabeta, R. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 15D, 16A (*haz*)

$C_2H_3NbO_4$ IC-003087

(Acetato-*O*)dioxoniobium(*V*), 11CI

[10493-29-5]

$NbO_2(OAc)$

M 183.9

Synth. by reaction of excess HOAc and $NbCl_5$ in CCl_4. White solid. Ir ν_{Nb-O} 835 cm^{-1}.

Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1985, **24**, 761 (*synth, ir*)

$C_2H_3NiO_2^{\oplus}$ IC-003088

Acetatonickel(*II*)(1+)

$[NiOAc]^{\oplus}$

M 117.7 (ion)

Formed, undoubtedly hydrated, in aq. $Ni^{2\oplus}/OAc^{\ominus}$ solns.

Fuentes, R. *et al, Inorg. Chem.*, 1975, **14**, 1837.
Benson, A. *et al, Inorg. Chem.*, 1976, **15**, 1212.

$C_2H_3O_2Rb$ IC-003089

Rubidium acetate (RbOAc)

Acetic acid, rubidium salt, 8CI. Ethanoic acid, rubidium salt

[563-67-7]

RbOAc

M 144.5

Prepd. by slow neutralisation of Rb_2CO_3 with HOAc in aq. soln. Commercially available. Hygroscopic, colourless monoclinic cryst. V. sol. H_2O (86 g per 100 cm^3 at 45°; 89 g per 100 cm^3 at 99°). Mp 246°.

Gmelin Handbook Inorg. Chem., Syst. No. 24, 1955, 228 (*rev, bibl*)
Donaldson, J.D., *Spectrochim. Acta*, 1965, **21**, 275 (*ir*)
Hatibarua, J. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 3099 (*struct, polymorph*)

$C_2H_3O_2Tl$ IC-003090

Thallium(*I*) acetate

Thallium(I) *ethanoate. Acetatothallium*

[563-68-8]

TlOAc

M 263.4

Obt. by reaction of Tl_2CO_3 or TlOH with AcOH. Used extensively in org. synth., in heavy liq. for gravity conc. of ores. Hygroscopic, colourless, light-sensitive monoclinic cryst. (EtOH). V. sol. H_2O; mod. sol. EtOH. Mp 131°.

▷ V. toxic. AJ5425000.

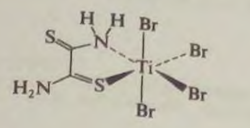
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, **2**, 884.
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1150; 1982, **10**, 393; 1984, **11**, 294 (*uses*)
Taylor, E.C. *et al, Acc. Chem. Res.*, 1970, **3**, 338 (*reactions*)
Caranoni, C. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **271**, 673 (*struct*)
Compr. Organomet. Chem., Pergamon, Oxford, 1982, **7**, 465 (*reactions*)

$C_2H_4Br_4N_2S_2Ti$ IC-003091

Tetrabromo(ethanedithioamide-N^1,S^2)titanium(*IV*), 11CI

Tetrabromo(dithiooxamide)titanium(IV)

[84204-16-0]



M 487.6

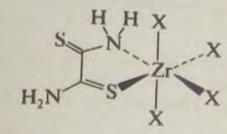
Synth. by adding a suspension of dithiooxamide in CH_2Cl_2 to $TiBr_4$ in CH_2Cl_2. Sol. MeCN. Dipole moment 6.9D, non-electrolyte in MeCN.

Martinez, M.C. *et al, Acta Cient. Compostelana*, 1981, **18**, 15; 1983, **20**, 15 (*synth, ir, uv-vis, props*)

$C_2H_4Br_4N_2S_2Zr$ IC-003092

Tetrabromo(ethanedithioamide-N^1,S^2)zirconium(*IV*), 11CI

Tetrabromo(dithiooxamide-N^1,S^2*)zirconium*(IV). *Zirconium*(IV) *bromide dithiooxamide*



X = Br

M 531.0

Octahedral.

cis-form [95861-50-0]

Synth. by mixing solns. of $ZrBr_4$ and ethanedithioamide in CH_2Cl_2.

Martinez, M.C. *et al, Acta Cient. Compostelana*, 1983, **20**, 5 (*synth, ir, uv*)

C_2H_4ClF IC-003093

1-Chloro-1-fluoroethane, 9CI

Ethylidene chlorofluoride. Fluorocarbon 151a

[1615-75-4]

$H_3CCHClF$

M 82.5

Gas or liq. at r.t. Bp 16.1-16.2°.

▷ KH7784000.

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1936, **58**, 887 (*synth*)

C_2H_4ClF IC-003094

1-Chloro-2-fluoroethane, 9CI

Ethylene chlorofluoride. Fluorocarbon 151

[762-50-5]

$ClCH_2CH_2F$

M 82.5

Liq. d^{23} 1.176. Bp 53.2°.

▷ KH7785000.

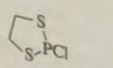
Swarts, F., *Chem. Zentralbl.*, 1903, **1**, 13.
McCombie, H. *et al, Nature (London)*, 1946, **158**, 382.
Beaty, T., *Acta Pol. Pharm.*, 1955, **12**, 223; *CA*, **50**, 17042.
Edgell, W.F. *et al, J. Am. Chem. Soc.*, 1955, **77**, 4899 (*synth*)
Robert, D.V. *et al, Tetrahedron*, 1973, **29**, 1877 (*synth*)
Middleton, W.J. *et al, J. Org. Chem.*, 1975, **40**, 574 (*synth*)

$C_2H_4ClPS_2$ IC-003095

2-Chloro-1,3,2-dithiaphospholane, 9CI, 8CI

Ethylene phosphorochloridodithioite. Ethylene chlorodithiophosphite

[4669-51-6]



M 158.6

Pungent liq. Easily hydrol. and oxidised. Bp_{10} 100°, $Bp_{0.5}$ 80°. n_D^{20} 1.6870.

2-Oxide: [35437-33-3]. *S,S-Ethylene phosphorochloridodithioate*

$C_2H_4ClOPS_2$ M 174.6

No phys. props. reported.

2-Sulfide: [34303-19-0]. *Ethylene phosphorochloridotrithioate*

$C_2H_4ClPS_3$ M 190.6

Cryst. (Et_2O/pet. ether). Mp 45°.

Kovalev, L.S. *et al, Zh. Obshch. Khim.*, 1968, **38**, 2277; *J. Gen. Chem. USSR (Engl. Transl.)*, 1968, **38**, 2203 (*synth*)
Lee, J.D. *et al, Acta Crystallogr., Sect. B*, 1971, **27**, 1055 (*sulfide, cryst struct*)
Peake, S.C. *et al, J. Chem. Soc., Perkin Trans. 2*, 1972, 380 (*synth, derivs, P-31 nmr, pmr*)
Ishmaeva, E.A. *et al, Zh. Obshch. Khim.*, 1972, **42**, 2642; *J. Gen. Chem. USSR (Engl. Transl.)*, 1972, **42**, 2633 (*sulfide, stereochem*)
Schultz, G.Y. *et al, Tetrahedron*, 1974, **30**, 2365 (*ed*)
Gonbeau, D. *et al, J. Mol. Struct.*, 1983, **98**, 109 (*pe, struct, cmr*)
Davidson, G. *et al, Spectrochim. Acta, Part A*, 1983, **39**, 419 (*ir, raman*)
Plyamovatyi, A.Kh. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1986, 1116; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1986, 1011 (*conform*)
Shagidullin, R.R. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1986, 1793; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1986, 1627 (*ir, raman*)

$C_2H_4Cl_2$ IC-003096

1,1-Dichloroethane, 9CI

Ethylidene chloride. R150a

[75-34-3]

H_3CCHCl_2

M 98.9

Manuf. by catalysed reaction of vinyl chloride with HCl. Solvent, used also in manuf. of H_3CCCl_3. Liq. d_4^{20} 1.175. Fp −98°. Bp 57.3°. n_D^{15} 1.4198.

▷ Mod. toxic by inhalation, OES 810 mg m^{-3}. An exp. teratogen. Flammable, flash p. 6°. KI0175000.

D'Ans, J. *et al, J. Prakt. Chem.*, 1909, **80**, 310 (*synth*)
Miyajima, G. *et al, J. Phys. Chem.*, 1971, **75**, 331 (*cmr*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 278.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1148.

$C_2H_4Cl_2$ IC-003097

1,2-Dichloroethane, 9CI

Ethylene dichloride. Ethylene chloride. Dutch oil. R 150

[107-06-2]

$ClCH_2CH_2Cl$

M 98.9

Manuf. by chlorination, or oxychlorination (O_2 + HCl), of ethylene. Industrial solv., intermediate for vinyl chloride manuf. Liq. d_4^{20} 1.252. Fp −35.3°. Bp 83-84°. n_D^{20} 1.4443.

▷ Toxic, skin irritant. OES 40 mg m^{-3}. Exp. carcinogen and teratogen. Flammable, Flash p. 13°. KI0525000.

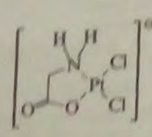
Bahr, H.A. *et al, Angew. Chem.*, 1930, **43**, 233; *CA*, **24**, 2717 (*synth*)
Simeral, L. *et al, J. Phys. Chem.*, 1973, **77**, 1590 (*cmr*)
Occupational Exposure Limits 1991, Health and Safety Executive, HMSO, London, 1991, EH40/91 (*haz*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 278.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1148.

IC-003098

$C_2H_4Cl_2NO_2Pt^{\odot}$

Dichloro(glycinato-*N,O*)platinate(*II*)(1−), 8CI

[24653-14-3]



M 340.0 (ion)
Probably square planar. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + glycine.

▷ TP2497180.

K salt: [17567-43-0].
Yellow cryst. (EtOH). Sol. H_2O.

Kieft, J.A. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 2561 (*ir*)
Erickson, L.E. *et al, J. Am. Chem. Soc.*, 1968, **90**, 6371 (*synth, pmr*)
Erickson, L.E. *et al, Inorg. Chem.*, 1978, **17**, 1701 (*cmr*)

IC-003099

$C_2H_4Cl_4N_2S_2Zr$

Tetrachloro(ethanedithioamide-N^1,S^2)zirconium(*IV*), 11CI

Tetrachloro(dithiooxamide-N^1,S^2*)zirconium*(IV). *Zirconium*(IV) *chloride dithiooxamide*

[95861-49-7]

As Tetrabromo(ethanedithioamide-N^1,S^2)zirconium(*IV*), IC-003092 with

X = Cl

M 353.2
Octahedral. Synth. by adding a soln. of ethanedithiooxamide in CH_2Cl_2 to a slurry of $ZrCl_4$ in CH_2Cl_2. White, readily hydrol. solid; non-electrolyte in MeCN. Sol. MeCN.

Martinez, M.C. *et al, Acta Cient. Compostelana*, 1983, **20**, 205 (*synth, ir, uv*)

IC-003100

$C_2H_4FO_7V^{\odot}$

Diaquafluoro(oxalato)oxovanadate(*IV*)(1−)

Diaqua[ethanedioato(2−)-O,O′]fluorooxovanadate(IV)(*1−*), *10CI*

M 209.9 (ion)
Octahedral anion.

NH_4 salt: [76333-69-2].
Synth. by adding NH_4HF_2 to a soln. of V_2O_5 in aq. oxalic acid.

Pyridinium salt: Synth. by dissolving $(PyH)_2[VOCl_4]$ in 40% HF then adding oxalic acid. Blue solid (40% HF).

Edwards, A.J. *et al, Bull. Soc. Chim. Fr.*, 1975, 2015 (*synth, cryst struct*)
Sengupta, A.K. *et al, Indian J. Chem., Sect. A*, 1980, **19**, 914 (*synth, ir*)

IC-003101

$C_2H_4F_2$

1,1-Difluoroethane, 9CI

Ethylidene fluoride. Fluorocarbon 152a

[75-37-6]

H_3CCHF_2

M 66.0
Derived by addition of HF to acetylene. Gas. Fp −117°. Bp −24.7°. Physiologically almost inert.

▷ Flammable; toxic fumes evolved as thermal dec.. KI1410000.

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1936, **58**, 890 (*synth*)
Nagase, S. *et al, Bull. Chem. Soc. Jpn.*, 1966, **39**, 219 (*synth*)
Akramkhodzhaev, A. *et al, CA*, 1973, **79**, 137533 (*synth*)
Brandwood, M. *et al, J. Fluorine Chem.*, 1975, **5**, 521 (*synth*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1254.

IC-003102

$C_2H_4F_2$

1,2-Difluoroethane, 9CI

Ethylene difluoride. Fluorocarbon 152

[624-72-6]

FH_2CCH_2F

M 66.0
Volatile liq. Bp 25-27° (30.7°) (10.5°).

Brandwood, M. *et al, J. Fluorine Chem.*, 1975, **5**, 521 (*synth*)
Middleton, W.J., *J. Org. Chem.*, 1975, **40**, 574 (*synth*)
Burdon, J. *et al, Tetrahedron*, 1976, **32**, 1041 (*synth*)
Vitus, D.M., *Diss. Abstr. Int., B*, 1977, **37**, 3985; *CA*, **86**, 170730 (*conformn*)

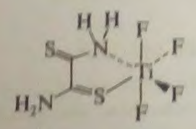
IC-003103

$C_2H_4F_4N_2S_2Ti$

(Ethanedithioamide-N^1,S^2)tetrafluorotitanium(*IV*), 11CI

(*Dithiooxamide-*N^1,S^2)*tetrafluorotitanium*(IV). *Titanium*(IV) *fluoride dithiooxamide*

[84640-40-4]



M 244.0
Synth. by adding TiF_4 in CH_2Cl_2 to a suspension of the ligand in CH_2Cl_2. Sol. MeCN. Non electrolyte in MeCN.

Martinez, M.C. *et al, Acta Cient. Compostelana*, 1981, **18**, 15; *CA*, **98**, 82711t (*synth, ir, uv-vis*)

IC-003104

$C_2H_4F_4S$

(Ethylidene)tetrafluorosulfur

Ethylidenesulfur tetrafluoride

[81553-81-3]

$H_3CCH{=}SF_4$

M 136.1

Synth. from $H_3CC{\equiv}COR$ + $SClF_5$ (multistage). Colourless liq. or gas, slowly dec. at 25° in glass. Mp < −120°. Bp 27°.

Paetter, B. *et al, Inorg. Chem.*, 1982, **21**, 3147 (*synth, pmr, F-19 nmr, ir, ms*)

IC-003105

$C_2H_4FeO_6$

Diaqua(oxalato)iron(*II*)

Diaqua[ethanedioato(2−)-O,O′]iron(II). *Iron*(II) *oxalate dihydrate*

[6047-25-2]

$FeC_2O_4.2H_2O$

M 179.8
Exists as α-form (monoclinic, more thermodynamically stable) and β-form (orthorhombic). Both forms have identical ir. Obt. by recryst. of $Fe(C_2O_4)$ from H_2O or $Fe^{2\oplus}$ + oxalate in water. Photographic developer. Pigment in glasses, plastics and paint. Scale preventor. Light-sensitive, hygroscopic yellow cryst. (H_2O). Sol. acids; insol. H_2O. μ_{eff} = 5.11μ_B (300K).

▷ Toxic, irritant.

[15703-34-9]

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1930, **B3**, 532 (*rev, bibl*)
Deyrieux, R. *et al, Bull. Soc. Chim. Fr.*, 1969, 2675 (*struct, allotropes*)

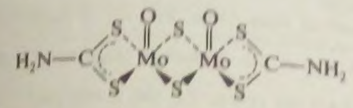
IC-003106

$C_2H_4Mo_2N_2O_2S_6$

Bis(dithiocarbamato)dioxodi-μ-thiodimolybdenum(*V*)

*Bis(carbamodithioato-*S,S′*)dioxodi-μ-thioxodimolybdenum, 11CI*

[90065-77-3]



M 472.3
Square pyramidal coordination. Interatomic distances: Mo—S 246.0; Mo—S_{bridge} 232.4; Mo—O 167.7; Mo—Mo 282.0 pm. Yellow-brown cryst. + 2MeCN (MeCN). Loses MeCN of crystallisation in air.

Howlader, N.C. *et al, Inorg. Chem.*, 1984, **23**, 1811 (*cryst struct, synth, uv, ir, electrochem*)

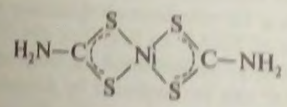
IC-003107

$C_2H_4N_2NiS_4$

Bis(dithiocarbamato)nickel(*II*), 8CI

*Bis(carbamodithioato-*S,S′*)nickel, 9CI. Nickel*(II) *dithiocarbamate*

[13985-94-9]



M 243.0
Square planar. Dark green cryst. (EtOH).

Bis-Py complex:
$C_{12}H_{14}N_4NiS_4$ M 401.2
Grass green cryst. Sol. Me_2CO. Presumed 6-coordinate. Dec. on keeping to $NiPy_2(SCN)_2$.

Bis(4-methylpyridine) complex:
$C_{14}H_{18}N_4NiS_4$ M 429.2
Green cryst. μ_{eff} = 2.9μ_B.

Delepine, M., *Bull. Soc. Chim. Fr.*, 1908, 643 (*synth*)

Jorgensen, C.K., *J. Inorg. Nucl. Chem.*, 1962, **24**, 1571 (*uv-vis, mcd*)
Nakamoto, K. *et al, J. Chem. Phys.*, 1963, **39**, 423 (*ir*)
Gaspani, G.P. *et al, Acta Crystallogr.*, 1967, **23**, 384 (*cryst struct*)
Cotocorvanis, D. *et al, Inorg. Chem.*, 1967, **6**, 2047 (*synth, ir, complexes*)
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1968, C2, 987 (*rev*)

IC-003108

$C_2H_4N_2O_2S_2$

1,2-Hydrazine bis(monothioformic acid)

1,2-Hydrazinedicarbothioic acid

$HSC(O)NHNHC(O)SH$

M 152.1
Isol. as ester.

S,S′-Di-Me ester: [89166-56-3].
$C_4H_8N_2O_2S_2$ M 180.2
From N_2H_4 + COS + NaOMe followed by addn. of MeI. Colourless cryst., stable at 25°. Sol. EtOH, Et_2O, DMSO. Mp 173°.

Nachbaur, E. *et al, Monatsh. Chem.*, 1964, **95**, 779 (*deriv, synth, ir*)
Gattow, G. *et al, Z. Anorg. Allg. Chem.*, 1986, **533**, 109 (*deriv, synth, ir, pmr, cmr*)

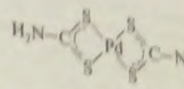
IC-003109

$C_2H_4N_2PdS_4$

Bis(dithiocarbamato)palladium(*II*)

*Bis(carbamodithioato-*S,S′*)palladium, 10CI*

[52587-19-6]



M 290.7
Yellow cryst. Sol. $CHCl_3$, Me_2CO, DMF. Mp 206° dec.

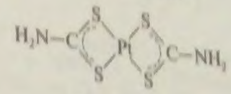
Nakamoto, K. *et al, J. Chem. Phys.*, 1963, **39**, 423 (*synth, ir*)
Ahmed, M. *et al, J. Electroanal. Chem.*, 1980, **110**, 335 (*electrochem*)
Sceney, C.G. *et al, Inorg. Nucl. Chem. Lett.*, 1974, **10**, 323 (*synth, ir*)

IC-003110

$C_2H_4N_2PtS_4$

Bis(dithiocarbamato)platinum(*II*)

*Bis(carbamodithioato-*S,S′*)platinum*(II)



M 379.4
Probably square planar. Prototype of other dithiocarbamates. Synth. from $NH_4(NH_2CS_2)$ + Pt salt.

Nakamoto, K. *et al, J. Chem. Phys.*, 1963, **39**, 423 (*synth, ir*)

IC-003111

$C_2H_4N_2S_4Zn$

Bis(dithiocarbamato)zinc

*Bis(carbamodithioato-*S,S′*)zinc. Zinc dithiocarbamate*

[18984-88-8]

$[H_2NC(S)S]_2Zn$

M 249.7
Antioxidant, fungicide. Solid.

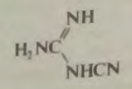
Bernard, M.A. *et al, Bull. Soc. Chim. Fr.*, 1969, 3064, 3066, 3069 (*synth, thermal anal, cryst struct*)
Pilipenko, A.T. *et al, CA*, 1970, **73**, 135492 (*ir*)

$C_2H_4N_4$ IC-003112

Cyanoguanidine, 9CI

Dicyandiamide

[461-58-5]



M 84.0

Has also been formulated as $(H_2N)_2C{=}NC{\equiv}N$. Formed from cyanamide and $OH^{\ominus}$. Commercially available. Used in plastics and pharmaceutical industries and in heterocyclic synth. Prisms (H_2O). Mod. sol. H_2O, EtOH, liq. NH_3; insol. Et_2O, C_6H_6. Mp 209.5°. Forms salts with many metals. The mono-K salt is sol. in H_2O and the di-K salt spar. sol.

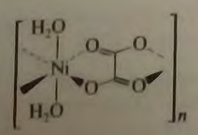
Franklin, E.C., *J. Am. Chem. Soc.*, 1922, **44**, 501.
Braham, J.M., *J. Am. Chem. Soc.*, 1923, **45**, 824 (*synth*)
Hughes, E.W., *J. Am. Chem. Soc.*, 1940, **62**, 1258 (*struct*)
Inorg. Synth., 1950, **3**, 43 (*synth*)
Jones, W.J. *et al*, *Trans. Faraday Soc.*, 1959, **55**, 193 (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 229.
Beynon, J.H. *et al*, *Org. Mass Spectrom.*, 1968, **1**, 169 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **7**, 291, 299.
Hirshfeld, F.L. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 406 (*struct*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 374.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 988.

$C_2H_4NiO_6$ IC-003113

Diaqua(oxalato)nickel(*II*)

Nickel(II) *oxalate dihydrate. Diaqua[ethanedioato(2−)-O,O′]nickel*(II), *9CI*

[6018-94-6]



M 182.7

Polymeric chain struct. with octahedral Ni. Synth. from Hexaaquanickel(*II*)(2+), IC-019897 + $C_2O_4^{2\ominus}$. Greenish-white solid. Insol. H_2O; sol. acids, NH_3 aq. Antiferromagnetic. Loses $2H_2O$ at 150°, dec. below 320° to Ni + CO_2. Many studies of thermolysis.

[55703-37-2, 55703-38-3]

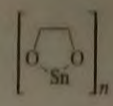
Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1435.
Sharov, V.A. *et al*, *Koord. Khim.*, 1977, **3**, 1865 (*ω, magnetism*)
Kondratov, O.I. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 72 (*ir, raman*)

$C_2H_4O_2Sn$ IC-003114

(1,2-Ethanediolato)tin

2,2-Didehydro-1,3,2-dioxastannolane, 9CI. Tin(II) *ethyleneglycoxide*

[68921-71-1]



M 178.7

Polym. struct. is a 3-D network of linked Sn(*II*) ethylene glycol chelates. Synth. by refluxing $Sn(OH)_2$ in ethylene glycol. Cryst.

[28205-52-9]

Fenton, D.E. *et al*, *Inorg. Chim. Acta*, 1970, **4**, 235 (*synth*)
Nesper, R. *et al*, *Z. Naturforsch., B*, 1982, **37**, 1144 (*synth, cryst struct*)

$C_2H_2O_6U$ IC-003115

Bis(formato-*O*)dioxouranium(*VI*)

Uranyl(VI) *formate*

[16984-59-1]

$$UO_2(OOCH)_2$$

M 360.0

Studied for isotope separation by laser photochemical redn. of selected isotope. Usually obt. as hydrate. Np, Pu analogues isostructural. Dec. to U_3O_8 at 690°.

Monohydrate: [36936-45-5].
$C_2H_4O_7U$ M 378.0
Bright yellow cryst. Sol. H_2O, HCOOH. 7-Coord. pentagonal bipyramid with U=O 176 pm. Loses H_2O at 170°. Ir ν_{UOU} 930as, ν_{OUO} 864s cm^{-1}. Photosensitive to vis., uv, X-radiation.

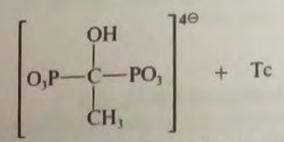
[20002-64-6, 58797-81-2]

Buttres, G.D. *et al*, *J. Chem. Soc. A*, 1968, 1272 (*synth, thermal dec*)
Bideau, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **271**, 225 (*thermal dec*)
Claudel, B. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **280**, 169.
Claudel, B. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 769 (*photo dec*)
Mentzen, B.F. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1848 (*ir, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 55 Suppl. Vol., 1983, **C13**, 97 (*rev*)
Anan'ev, A.V. *et al*, *Sov. Radiochem.* (*Engl. Transl.*), 1983, **25**, 331.
U.S. Pat., 4 439 404, (1984); *CA*, **100**, 217682 (*use*)

$[C_2H_4O_7P_2Tc^{4\ominus}]$ IC-003116

Ethane-1-hydroxy-1,1-diphosphonate technetium complex

Etidronate - Tc. EHDP - Tc. HEDP - Tc. Technetium-EHDP



This system contains a number of ill-defined complexes, whose nature depends on the method of preparation. May include a Tc—Sn heteropolynuclear species. Synth. by reduction of $TcO_4^{\ominus}$ by Sn(*II*) or $BH_4^{\ominus}$, or electrochemically. Mainly used for bone imaging. Rather labile - HEDP can be displaced by gluconate.

McRae, J. *et al*, *J. Nucl. Med.*, 1976, **17**, 208 (*ligand exchange*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, Suppl. Vol. 2, 1983, 210.
Zodda, J.P. *et al*, *Appl. Radiat. Isot.*, 1986, **37**, 345 (*synth, characterisation*)
Pinkerton, T.C. *et al*, *Nucl. Med. Biol.*, 1986, **13**, 49 (*synth, chromatog, biodistribn*)
Mikelsons, M.V. *et al*, *Appl. Radiat. Isot.*, 1987, **38**, 569 (*ir, raman*)
DeGroot, G.J. *et al*, *Appl. Radiat. Isot.*, 1987, **38**, 611 (*synth, chromatog*)

Nieuwland, R.J.A. *et al*, *Appl. Radiat. Isot.*, 1989, **40**, 153 (*synth, characterisation*)
Tji, T.G. *et al*, *Appl. Radiat. Isot.*, 1990, **41**, 17 (*synth, characterisation*)

$C_2H_4O_7V$ IC-003117

Aqua[ethanedioato(2−)-*O,O′*]oxovanadium(*IV*) monohydrate, 11CI

Diaqua[ethanedioato(2−)-O,O′]oxovanadium(IV), *10CI. Aqua(oxalato)oxovanadium*(IV) *monohydrate*

[81211-28-1]

$$[VO(OH_2)(O_2CCO_2)].H_2O$$

M 190.9

Formulation uncertain. Synth. from V_2O_5 and $H_2C_2O_4$ in boiling H_2O. Dark blue solid. Paramagnetic; μ_{eff} = 1.57μ_B (300K), 1.41μ_B (80K).

[13682-84-3, 66219-79-2]

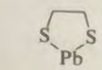
Sathyanaryana, D.N. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 297 (*synth*)
Povarova, P.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1977, **22**, 537 (*magnetism, uv-vis*)
Udapa, M.R., *Thermochim. Acta*, 1981, **51**, 169 (*thermal anal*)

$C_2H_4PbS_2$ IC-003118

Ethane-1,2-dithiolatolead

Lead ethane-1,2-dithiolate

[86860-88-0]



M 299.3

Cryst. comprise polymeric two-dimensional sheets. Light-yellow cryst. (MeOH/MeCN).

Dean, P.A.W. *et al*, *Inorg. Chem.*, 1985, **24**, 3594 (*synth, cryst struct*)

$C_2H_4S_2$ IC-003119

1,3-Dithietane, 9CI

[287-53-6]

M 92.1

Dimer of Thioformaldehyde, IC-002519. Cryst. (pentane) with powerful obnoxious odour. Mp 105-106°.

1-Oxide: [58816-63-0].
C_2H_4OS M 76.1
Cryst. (CCl_4). Mp 71-73.5°.
1,1-Dioxide: [60743-07-9].
$C_2H_4O_2S$ M 92.1
Mp 140-142°.
Tetroxide: [21511-46-6]. *Disulfene. 1,3-Dithietane 1,1,3,3-tetroxide*
$C_2H_4O_4S_2$ M 156.1
Synth. from $MeSO_2Cl$ + Me_3N in THF at −20°. Brown cryst. (DMSO or DMF). Base sensitive, stable to acids incl. hot conc. H_2SO_4. Sl. sol. most solvs. Mp >280° dec.

Opitz, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 73 (*synth, ir, nmr, tetroxide*)
Block, E. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 3119 (*synth, spectra*)

$C_2H_5AlO_4$ IC-003120

Aluminium acetate hydroxide (Al(OAc)(OH)$_2$)

Aluminium bis(hydroxide) acetate. Aluminium bis(hydroxide) ethanoate

[7360-44-3]

$$Al(OH)_2OAc$$

M 120.0

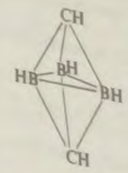
Synth. from $Al_2(SO_4)_3$, HOAc and $CaCO_3$. Used in pharmaceutical industry as detergent, antiseptic, and astringent. With HOAc, constitutes Burrow's soln. White solid.

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 202.

$C_2H_5B_3$ IC-003121

1,5-Dicarbapentaborane(5), 10CI

[20693-66-7]



M 61.4

closo-. Colourless gas. Mp −126.4°. Bp −3.7°.

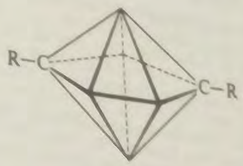
Shapiro, I. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 3837 (*ir, ms, nmr*)
Ditter, J. *et al*, *Inorg. Chem.*, 1970, **9**, 889 (*synth*)

$C_2H_5B_5Li_2$ IC-003122

μ-2,4-Dicarbaheptaborane(7)-2,4-diyldilithium, 9CI

2,4-Dilithio-2,4-dicarbaheptaborane(7)

[38386-34-4]



R = Li

M 96.9

closo-. Precursor for the preparation of σ-substituted derivatives eg. for polymer formation. Sol. Et_2O, C_6H_6.

Olsen, R. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 5072 (*synth*)
Kesting, R. *et al*, *J. Appl. Polym. Sci.*, 1970, **14**, 2525 (*synth*)

$C_2H_5BrFeN_3O_2S$ IC-003123

Bromo(ethanethioamide-*S*)dinitrosyliron

[52394-47-5]

$$FeBr(NO)_2[S{=}C(NH_2)CH_3]$$

M 270.8

Tetrahedral at Fe. Originally formulated with chelating thioamide; later proposed unidentate *S*-coordination. Synth. from $[Fe(NO)_2Br]_2$ with thioamide. Sol. THF; insol. pet. ether. Fp 51°.

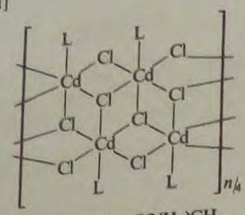
Birchall, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2521 (*ir, esr, mössbauer*)
Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **358**, 271 (*synth, ir*)

$C_2H_5CdCl_2NS$ IC-003124

Dichloro(thioacetamide-*S*)cadmium(*II*)

Di-μ-chlorobis[thioacetamide(chloro)cadmium]. Cadmium(II) *chloride bis(thioacetamide)*

[68831-48-1]



L = $S{=}C(NH_2)CH_3$

M 258.4

Solid state struct. comprises infinite double chains of octahedral Cd connected by bridging Cl. White needles (aq. EtOH).

Rolies, M.M. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 3216 (*synth, cryst struct*)

C_2H_5Cl IC-003125

Chloroethane

***Ethyl chloride*, USAN.** *R 160. Other proprietary names*

[75-00-3]

H_3CCH_2Cl

M 64.5

Manuf. by catalysed addition of HCl to ethylene. Used in manuf. of $PbEt_4$ and ethylcellulose. Aerosol refrigerant. Topical anaesthetic. Volatile liq. or gas at r.t. Spar. sol. H_2O. d_6^6 0.917. Fp −142.5° (−139°). Bp 12.5° (13.1°).

▷ Mild irritant. Mod. toxic vapour, TLV 2,600. Highly flammable, flash p. −50°. KH7525000.

Groves, C.E., *Justus Liebigs Ann. Chem.*, 1874, **174**, 372.
Krüger, F., *J. Prakt. Chem.*, 1876, **14**, 195.
Norris, J.F. *et al, J. Am. Chem. Soc.*, 1924, **46**, 753 (*synth*)
U.S. Pat., 1 920 246, 1 920 846, (1933); *CA*, **27**, 4818 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **5**, 714 (*rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 3108.
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 53.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 244.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1607.

$C_2H_5ClO_3PV$ IC-003126

Chloro[monoethylphosphito(2−)-*O*']vanadium(*III*), 11Cl

[85626-50-2]

$VCl[PO_2(OEt)]$

M 194.4

Polymeric; detail unknown. Synth. from VCl_3 and $HP(O)(OEt)_2$ in C_6H_6 or at 110-120° in absence of solvent. Brown solid. Sol. C_6H_6. A number of similar compds. known.

Puri, D.M. *et al, Proc. Natl. Acad. Sci., India, Sect. A*, 1981, **51**, 507; *CA*, **98**, 190595s (*synth, ir, magnetism*)

$C_2H_5Cl_2NNiS$ IC-003127

Dichloro(thioacetamide)nickel(*II*)

Dichloro(ethanethioamide-S)nickel, 9CI. Nickel(II) *chloride thioacetamide complex*

[36088-55-8]

$NiCl_2(S{=}CNH_2CH_3)$

M 204.7

Possibly 6-coord. polymer. Yellow-green cryst. Sol. MeCN. $\mu_{eff} = 2.62\mu_B$. Antiferromagnetic coupling postulated. Non-electrolyte.

Iyengov, R.R. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 1088 (*synth, magnetism, uv-vis, ir*)

$C_2H_5Cl_2NbO_2$ IC-003128

Dichloro(ethoxy)oxoniobium(*V*), 11Cl

[92834-30-5]

$NbOCl_2(OEt)$

M 224.8

Tetrahedral. Synth. from $NbCl_5$ and EtOH.

Nisel'son, L.A. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1984, **29**, 1289 (*synth, ir*)

$C_2H_5Cl_2OP$ IC-003129

Ethyl phosphorodichloridite, 9CI, 8CI

Ethyl dichlorophosphite. Dichloroethoxophosphorus(III)

[1498-42-6]

$EtOPCl_2$

M 146.9

Fuming liq. d_4^{20} 1.29. Bp 116-118°, Bp_{18} 28-30°. n_D^{20} 1.4730.

▷ Violently hydrol. by H_2O. Highly irritant and corrosive.

Cook, H.G. *et al, J. Chem. Soc.*, 1949, 2921 (*synth, props*)
Schwarz, R. *et al, Chem. Ber.*, 1957, **90**, 952 (*synth*)
Fluck, E. *et al, Z. Anorg. Allg. Chem.*, 1961, **307**, 113 (*P-31 nmr*)
Steyermark, P.R., *J. Org. Chem.*, 1963, **28**, 586.
Armour, M.A. *et al, J. Chem. Soc., Perkin Trans. 2*, 1975, 1185 (*synth*)
Gazizov, T.Kh. *et al, Zh. Obshch. Khim.*, 1977, **47**, 1234; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1977, **47**, 1137 (*synth*)
Mikaya, A.I. *et al, Zh. Obshch. Khim.*, 1982, **52**, 1998; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1982, **52**, 1776 (*ms*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 6th Ed., Van Nostrand-Reinhold, 1984, 672.

$C_2H_5Cl_2OSb$ IC-003130

Dichloroethoxystibine, 8CI

Dichloroethoxoantimony

[25705-43-5]

$EtOSbCl_2$

M 237.7

Platelets (CCl_4). Sol. EtOH, spar. sol. CCl_4, insol. Et_2O. Mp 116-117°. Bp_{10} 125-127°.

Arbuzov, B.A. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 390; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1976, 370 (*synth, ir*)
Binder, G.E. *et al, Z. Anorg. Allg. Chem.*, 1980, **471**, 121; 1983, **507**, 163 (*cryst struct, ms, ir, raman*)

$C_2H_5Cl_2OTi$ IC-003131

Dichloroethoxytitanium(*III*), 11Cl

[4055-63-4]

$TiCl_2OEt$

M 163.8

Polymeric. Synth. by adding $TiCl_3$ to soln. of triethyl orthoformate in heptane and heating under reflux. Green solid. Mp 300° dec.

Belg. Pat., 637 449, (1964); *CA*, **62**, 7889g (*use*)
Giannetti, E. *et al, Inorg. Chim. Acta*, 1983, **74**, 215 (*synth, ir, powder struct*)

$C_2H_5Cl_2OV$ IC-003132

Dichloroethoxyvanadium(*III*), 11Cl

Vanadium(III) *dichloride ethoxide*

[88092-81-3]

$VCl_2(OEt)$

M 166.9

Probably polymeric with bridging OEt groups. Synth. from VCl_3 and excess ethyl orthoformate. This is a general method for synthesising $VX_n(alkoxy)_{3-n}$ compds. Green solid. Mp 300° dec.

Giannetti, E. *et al, Inorg. Chim. Acta*, 1983, **74**, 215 (*synth, ir, powder struct*)

$C_2H_5Cl_2O_2P$ IC-003133

Ethyl phosphorodichloridate, 9CI, 8CI

Ethyl phosphoryl dichloride. Ethyl dichlorophosphate. Dichloroethoxooxophosphorus(V)

[1498-51-7]

$EtOP(O)Cl_2$

M 162.9

Colourless pungent liq. d_{25} 1.38. Bp 167°, Bp_{13} 58°. n_D^{20} 1.4342.

▷ TD4390000.

Saunders, B.C. *et al, J. Chem. Soc.*, 1948, 699 (*synth, tox*)
Grunze, H., *Chem. Ber.*, 1959, **92**, 850 (*synth, props*)
Williamson, M.P. *et al, J. Phys. Chem.*, 1968, **72**, 4043 (*pmr, bibl*)
Furlani, C. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 673 (*pe*)
Zverev, V.V. *et al, Zh. Obshch. Khim.*, 1979, **49**, 1737; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1979, **49**, 1522 (*pe*)
Bel'skii, V.E. *et al, Zh. Prikl. Spektrosk.*, 1980, **33**, 361; *CA*, **93**, 227847 (*ir*)
Appling, J.R. *et al, Org. Mass Spectrom.*, 1985, **20**, 343 (*ms*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1676.

$C_2H_5Cl_2O_2V$ IC-003134

Dichloroethoxyoxovanadium(*V*), 11Cl

[1801-77-0]

$VOCl_2(OEt)$

M 182.9

Tetrahedral. Synth. e.g. from $VOCl_3$ + Et_3SiOEt and an amine. Polym. and copolym. catalyst for olefins. Colourless moisture-sensitive liq. $Bp_{1.25}$ 52°.

Mittal, R.K. *et al, Z. Anorg. Allg. Chem.*, 1964, **332**, 189 (*synth from* $VO(OEt)_3$)
Gervais, D. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 3679 (*synth via NaOEt, uv-vis, props, magnetism*)
Preuss, F. *et al, Z. Naturforsch., B*, 1985, **40**, 1040 (*reactions*)
Ger. Pat., 3 447 290, (1986); *CA*, **105**, 227023v (*synth via* $Et_3Si(OEt)$)
Japan. Pat., 61 115 916, (1986); *CA*, **105**, 153716z (*use*)

$C_2H_5Cl_3NO_3PS$ IC-003135

Ethyl (chlorosulfonyl)phosphorodichlorimidate, 9CI

[32755-55-8]

$ClSO_2N{=}PCl_2OEt$

M 260.4

Liq. Isom. in presence of Et_2O.

Roesky, H.W. *et al, Chem. Ber.*, 1971, **104**, 3204 (*synth, pmr, ir, P-31 nmr, props*)

$C_2H_5Cl_3OTi$ IC-003136

Trichloroethoxytitanium(*IV*), 11Cl

Titanium(IV) *chloride ethoxide*

[3112-67-2]

$EtOTiCl_3$ (C_{3v})

M 199.2

Monomeric in C_6H_6 and dioxan. A mixt. of $TiCl_4$ and $SiCl_3OEt$ slowly deposits cryst. of $TiCl_3OEt$; alternatively $TiCl_4$ and $Ti(OEt)_4$ react in C_6H_6 to yield the same product. Olefin polym. catalyst. Yellow solid. Mp 81°.

Bradley, D.C. *et al, J. Chem. Soc.*, 1963, 2101 (*synth*)
Feltz, A. *et al, Z. Anorg. Allg. Chem.*, 1964, **334**, 186 (*synth*)
Ger. Pat., 3 447 297, (1986); *CA*, **105**, 175282g (*synth*)

$C_2H_5Cl_4NO_2P_2$ IC-003137

Ethyl (dichlorophosphinyl)phosphorodichloroimidate, 10Cl

P,P-Dichloro-N-dichlorophosphinyl-P-ethoxyphosphazene. P,P-Dichloro-N-dichlorophosphinyl-P-ethoxyphosphine imide

[74308-16-0]

$Cl_2P(O)N{=}PCl_2OEt$

M 278.8

Liq. Readily isomerises.

Thomas, B. *et al, Z. Chem.*, 1980, **20**, 335 (*synth, P-31 nmr, props*)
Riesel, L., *Z. Chem.*, 1980, **20**, 98 (*synth*)

$C_2H_5Cl_4NbO$ IC-003138

Tetrachloroethoxyniobium(*V*), 11Cl

[5754-01-8]

$NbCl_4(OEt)$

M 279.7

Synth. from $NbCl_5$ and EtOH, or with $Nb(OEt)_5$ or with diethyl sulfite or acetyl chloride.

Kolditz, L. *et al, Z. Chem.*, 1965, **5**, 349 (*synth*)
Mehrotra, R.C. *et al, J. Less-Common Met.*, 1966, **10**, 348 (*synth*)
Nisel'son, L.A. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1984, **29**, 1289 (*synth, ir*)

C_2H_5F IC-003139

Fluoroethane, 9CI

Ethyl fluoride. Fluorocarbon 161

[353-36-6]

H_3CCH_2F

M 48.0

Gas with ethereal odour. Sol. EtOH, Et_2O; spar. sol. H_2O. Fp −143.2°. Bp −37.7°.

▷ Flammable. KI3650000.

Price, C.C., *J. Org. Chem.*, 1973, **38**, 615 (*pmr*)
Olah, G.A. *et al, J. Am. Chem. Soc.*, 1974, **96**, 925 (*synth*)

Saur, O. *et al*, *CA*, 1976, **84**, 23972 (*ir*)
Tan, H.S. *et al*, *Int. J. Mass Spectrom. Ion Phys.*, 1976, **21**, 297
Spoormaker, T. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1978, **97**, 135 (*cmr*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1747.

IC-003140

$C_2H_5F_2OP$

Ethyl phosphorodifluoridite, 9CI, 8CI

Ethyl difluorophosphite. Ethoxodifluorophosphorus(III)

[24933-27-5]

$EtOPF_2$

M 114.0
Ligand for Fe, Ni, and Ir. Gas or liq. d_4^{15} 1.09. Bp 23-24°. n_D^{25} 1.3280.

Binder, H. *et al*, *Z. Naturforsch., B*, 1972, **27**, 753 (*synth, P-31 nmr*)
Ivanova, Zh.M. *et al*, *Zh. Obshch. Khim.*, 1972, **42**, 2115; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1972, **42**, 2110 (*synth*)
Lines, E.L. *et al*, *Inorg. Chem.*, 1973, **12**, 2111 (*synth, ir, ms, pmr, F-19, P-31 nmr*)

IC-003141

$C_2H_6F_8FeN_2O_3P_2$

(Ethyl phosphorodifluoridite-*P*)dinitrosyl(phosphorous trifluoride)iron, 9CI

[52595-12-7]

$Fe(NO)_2(PF_3)[P(OEt)F_2]$

M 317.8
Tetrahedral at Fe. Obt. by alkylation of $[Fe(NO)_2(PF_3)(PF_2O)]^{\ominus}$, itself made from $OH^{\ominus}$ + $Fe(NO)_2(PF_3)_2$ in THF. Red. Mp −78°.

Kruck, T. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **402**, 16 (*synth, ir, ms*)
Nixon, J.F., *Adv. Inorg. Chem. Radiochem.*, 1985, **29**, 41 (*rev*)

IC-003142

$C_2H_5F_{14}FeOP_5$

(Ethyl phosphorodifluoridite)tetrakis(phosphorous trifluoride)iron

(Phosphorodifluoridous acid)tetrakis(phosphorus trifluoride) iron ethyl ester, 8CI

[22364-79-0]

$(F_3P)_4FePF_2OEt$

M 521.7
Trigonal bipyramidal. Synth. from $[Fe(PF_3)_4(PF_2O)_2]_2Ba$ in Et_2O + $Et_2O^{\oplus}$. Bright yellow mobile liq. Mp −45°. Bp 121°. $^1J_{PF}$ 1260 Hz.

Kruck, T. *et al*, *Chem. Ber.*, 1968, **101**, 3827 (*synth, nmr, ir, ms*)
Nixon, J.F., *Adv. Inorg. Chem. Radiochem.*, 1985, **29**, 41 (*rev*)

IC-003143

C_2H_5KO

Potassium ethoxide

Ethanol, potassium salt, 9CI. Ethyl alcohol, potassium salt, 8CI. Ethoxypotassium

[917-58-8]

KOEt

M 84.1
Synth. by dissoln. of K in EtOH. Commercially available. Strong base. Moisture-sensitive white powder. Reacts with H_2O to form EtOH and KOH. Dec. on heating in a series of complex reactions which involve H_2 and C_2H_4 evolution. Sol. EtOH. ΔH_f° −496 kJ mol^{-1}.

▷ Flammable.

Barthel, J. *et al*, *Electrochim. Acta*, 1971, **16**, 723 (*association in EtOH*)
Blanchard, J.M. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1974, **71**, 472 (*thermodynamics*)
Blanchard, J.M. *et al*, *J. Therm. Anal.*, 1976, **9**, 191 (*thermal dec*)
Javadi, N. *et al*, *Q. Bull. Fac, Sci., Tehran Univ.*, 1976, **7**, 135; *CA*, 1977, **87**, 29902 (*ir*)
Krachanov, Kh. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1979, **12**, 3 (*use*)

IC-003144

C_2H_5LiO

Lithium ethoxide

Ethanol, lithium salt, 9CI. Ethyl alcohol, lithium salt, 8CI. Ethoxylithium

[2388-07-0]

LiOEt

M 45.0
Prepd. by dissolution of Li metal in excess EtOH; isol. and purif. by vacuum sublimation. Component of polym. and dehydrochlorination catalysts. Nucleophilic substitution reagent. Lithiation reagent. Forms complexes with EtLi in hydrocarbon solvs. Colourless powder. Moisture sensitive. Reacts with H_2O to form LiOH and EtOH. Reacts with acidic protons to form the corresp. Li salts. Dec. on heating in a complex reaction giving H_2 and C_2H_4. Sol. EtOH (12.5 g per 100 cm^3 at 24°, 18.2 g per 100 cm^3 at 70°); spar. sol. heptane (0.26 g per 100 cm^3 at 26°), pentane, Et_2O. ΔH_f° −532 kJ mol^{-1}.

Siminov, A.P. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1961, **136**, 634 (*soln ir*)
Talalaeva, T.V. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1964, 638 (*synth*)
Bains, M.S., *CA*, 1965, **63**, 10706b (*synth, pmr*)
Kamienski, C.W. *et al*, *J. Org. Chem.*, 1965, **30**, 3498 (*soly*)
Brown, T.L. *et al*, *J. Organomet. Chem.*, 1965, **3**, 1 (*complex formn, ir, Li-7 nmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 612 (*use*)
Turova, N.Ya. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1970, 752 (*soly, props*)
Blanchard, J.M. *et al*, *J. Chim. Phys., Physicochim. Biol.*, 1974, **71**, 472 (*thermochem data*)
Blanchard, J.M. *et al*, *J. Therm. Anal.*, 1976, **9**, 191 (*thermal dec*)

IC-003145

C_2H_5NaO

Sodium ethoxide

Ethanol, sodium salt, 9CI. Ethyl alcohol, sodium salt, 8CI. Ethoxysodium

[141-52-6]

NaOEt

M 68.0
Synth by reaction of Na or Na/Hg with dry ethanol in an inert atm. (N_2 or Ar). Commercially available in soln. in denatured EtOH or as solid. Used widely as a catalyst and reagent in org. chem. Moisture-sensitive white powder. Reacts with H_2O forming EtOH and aq. NaOH.

▷ Flammable solid, corrosive.

Seubold, F.H., *J. Org. Chem.*, 1956, **21**, 156 (*ir*)
Blanchard, J.M. *et al*, *J. Therm. Anal.*, 1976, **9**, 191 (*thermal anal*)
Dubusc, M. *et al*, *Bull. Union Physiciens*, 1979, **74**, 351; *CA*, 1980, **92**, 180590 (*use*)
Gold, V. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1982, 1615 (*pmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3140A, 3140B (*haz*)

$C_2H_5Na_3O_8$

Trisodium hydrogen carbonate, dihydrate IC-003146

Sodium sesquicarbonate dihydrate. Carbonic acid, sodium salt (2:3), dihydrate, 8CI

[6106-20-3]

$Na_3H(CO_3)_2.2H_2O$

M 226.0
Manuf. from mineral ores by conventional extraction methods. Synth. by reaction of $NaHCO_3$ and Na_2CO_3 in excess H_2O, slowly cooled from 70°. Used in SO_2 removal from gas flues. Also used in the manuf. of Na_2CO_3. Colourless monoclinic cryst. Dec. on heating by CO_2 and H_2O loss forming Na_2CO_3. V. sol. H_2O (13 g per 100 cm^3 at 0°; 42 g per 100 cm^3 at 100°). ΔH_f° −2682 kJ mol^{-1}; ΔG_f° −2381 kJ mol^{-1}; S° 301 J K^{-1} mol^{-1}.

Mineral-form [15243-87-5]

Trona

Common in western USA; also found in e.g. southern Greenland, Kenya, Tibet, Iran. Colourless or off-white.

Novak, A. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1385 (*ir*)
Rupert, J.P., *J. Phys. Chem.*, 1965, **69**, 3059 (*thermodyn*)
Tomaszewski, E.P. *et al*, *Przem. Chem.*, 1965, **44**, 334; *CA*, **63**, 7869h (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1966, **3**, 1363 (*rev, bibl*)
Eugster, H.P., *Contrib. Geol.*, 1971, **10**, 49 (*rev, synth*)
Chois, C.S. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2874 (*struct*)

C_1H_5OTl

Thallium(*I*) ethoxide IC-003147

Ethoxythallium(I)

[20398-06-5]

TlOEt

M 249.4
Tetrameric in soln. with cubane-like struct. Obt. by reaction of Tl, TlOH or Tl_2O with EtOH. Used in homogeneous base-catalysed reactions in non-polar media. Sol. org. solvs.

▷ V. toxic. KM2940000.

Tetramer: Tetra-μ_3-ethoxytetrathallium
$C_8H_{20}O_4Tl_4$ M 997.7

Dahl, L.F. *et al*, *J. Inorg. Nucl. Chem.*, 1962, **24**, 357 (*synth*)
Bradley, D.C. *et al*, *Metal Alkoxides*, Academic Press, London, 1978 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1982, **10**, 395 (*use*)

$C_3H_6AgNO_3S$

Dimethylsulfide(nitrato)silver IC-003148

(Nitrato-O)[thiobis(methane)]silver, 10CI, 9CI. (Dimethylsulfide)silver nitrate. Silver nitrate (dimethyl sulfide)

[15171-27-4]

Me_2SAgNO_3

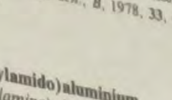
M 232.0
Useful starting material for synth. of alkoxy (*N*-alkylimino)methyl complexes. Cryst. (EtOH). Mp 120-123°.

Kubota, M. *et al*, *Inorg. Chem.*, 1966, **5**, 386 (*synth, ir*)
Minghetti, G. *et al*, *J. Organomet. Chem.*, 1973, **60**, C43 (*use*)
Minghetti, G. *et al*, *Inorg. Chem.*, 1975, **14**, 1974 (*synth*)
Bonati, F. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1976, **6**, 383 (*use*)

$C_2H_6AlBr_2N$

Dibromo(dimethylamido)aluminium IC-003149

Dibromo(dimethylamino)alane



Dimer

X = Br

M 230.8
Dimeric.

Dimer: [65929-91-1]. *Tetrabromobis[μ-(N-methylmethanaminato)]dialuminium, 10CI*
$C_4H_{12}Al_2Br_4N_2$ M 461.7
Synth. from H_2AlNMe_2 and $HgBr_2$. Colourless moisture sensitive plates. Mp 142-144°. Subl.$_{0.0001}$ 130°.

Ahmed, A. *et al*, *Z. Naturforsch., B*, 1978, **33**, 43 (*synth, cryst struct, ir, raman*)

$C_2H_6AlCl_2N$

Dichloro(dimethylamido)aluminium IC-003150

Dichloro(dimethylamino)alane

[26448-02-2]

As Dibromo(dimethylamido)aluminium, IC-003149 with

X = Cl

M 141.9
Dimeric.

Dimer: [56189-31-2]. *Tetrachlorobis[μ-(N-methylmethanaminato)]dialuminium, 9CI*
$C_4H_{12}Al_2Cl_4N_2$ M 283.9
From Me_2NAlH_2 and $HgCl_2$ or $(Me_2AlNMe_2)_2$ + $AlCl_3$.
Mp 237-238°. Subl.$_{0.0001}$ 104-105°.

Ruff, J.K., *J. Am. Chem. Soc.*, 1961, **83**, 1798 (*synth*)
Ehrlich, R., *Inorg. Chem.*, 1970, **9**, 146 (*synth, ms*)
Hoberg, H. *et al*, *Justus Liebigs Ann. Chem.*, 1971, **751**, 77 (*reactions*)
Bartke, T.C. *et al*, *Acta Chem. Scand., Ser. A*, 1975, **29**, 273 (*ref*)
Nöth, H. *et al*, *Z. Naturforsch., B*, 1975, **30**, 681 (*ir*)
Ahmed, A. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 3574 (*cryst struct*)
Cocco, L. *et al*, *J. Organomet. Chem.*, 1979, **179**, 1 (*cmr*)

$C_2H_6AlI_2N$

(Dimethylamido)diiodoaluminium IC-003151

(Dimethylamino)diiodoalane

As Dibromo(dimethylamido)aluminium, IC-003149 with

X = I

M 324.8
Dimeric.

Dimer: [65929-92-2]. *Tetraiodobis[μ-(N-methylmethanaminato)]dialuminium*
$C_4H_{12}Al_2I_4N_2$ M 649.7
Synth. from $HgAlNMe_2$ and HgI_2. Colourless moisture sensitive plates (C_6H_6/hexane 1:1). Dec. >100°.

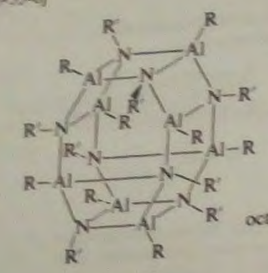
Ahmed, A. *et al*, *Z. Naturforsch., B*, 1978, **33**, 43 (*synth, ir, raman, cryst struct*)

C_2H_6AlN IC-003152

N-Ethyliminoalane

[Ethanaminato(2−)]hydroaluminium, 9CI

[27055-55-6]



octamer

R = H
R' = Et

M 71.0
Isol. as high polymer or oligomers (mainly octamer).

Octamer: [60910-00-1]. *Octakis[μ_3-[ethanaminato(2−)]]octahydrooctaaluminium, 9CI*

$C_{16}H_{48}Al_8N_8$ M 568.4
Mp 193°.

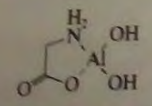
Nöth, H. *et al, Z. Naturforsch., B*, 1976, **31**, 697 (*synth, pmr, nmr, ms*)

$C_2H_6AlNO_4$ IC-003153

(Glycinato-*N,O*)dihydroxyaluminium, 9CI

Dihydroxyaluminium aminoacetate. Basic aluminium glycinate. Glycinal. Prodexin

[13682-92-3]



M 135.0
Antacid. Hydrate. Sol. dil. mineral acids.

[41354-48-7]

Gandhi, M.H., *Indian J. Chem.*, 1971, **6**, 182 (*synth*)
Japan. Pat., 21 756, (1971); *CA*, **75**, 80248y (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 671.

$C_2H_6AsCl_2N$ IC-003154

Dichloro(dimethylamino)arsine, 8CI

Dimethylarsenamidous dichloride, 9CI. Dichloro(dimethylamido)arsenic

[31012-32-5]

Me_2NAsCl_2

M 189.9
Liq. d_4^{21} 1.67. Bp_{30} 80-81°, Bp_{10} 51°. n_D^{20} 1.5556.

Vetter, H.-J. *et al, Z. Anorg. Allg. Chem.*, 1964, **330**, 233 (*synth*)
Schaeffer, C.D. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 3689 (*cmr*)
Durig, J.R. *et al, J. Mol. Struct.*, 1971, **10**, 427 (*pmr, ir, raman*)
Kober, F. *et al, Z. Chem.*, 1976, **16**, 232 (*ms*)
Osokin, D.Ya. *et al, Teor. Eksp. Khim.*, 1977, **13**, 64; *Theor. Exp. Chem. (Engl. Transl.)*, 1977, **13**, 45 (*nqr*)

$C_2H_6AsF_2N$ IC-003155

Difluoro(dimethylamino)arsine

Dimethylarsenamidous difluoride, 9CI. Difluoro(dimethylamido)arsenic

[758-23-6]

Me_2NAsF_2

M 156.9
Liq. Mp 2-4°. Bp_{42} 45-47°, Bp_{15} 30°. n_D^{20} 1.4461.

Olah, G. *et al, Can. J. Chem.*, 1960, **38**, 1431 (*synth*)
Singer, R.J. *et al, J. Fluorine Chem.*, 1971, **1**, 193 (*synth, pmr, F-19 nmr*)
Morse, J.G. *et al, Inorg. Chem.*, 1973, **12**, 2119 (*synth, ir, ms, pmr, F-19 nmr, props*)
Kober, F., *J. Fluorine Chem.*, 1973, **2**, 247; 1974, **4**, 65, 73 (*synth, ir, ms, F-19 nmr, uses*)

C_2H_6AuBrS IC-003156

Bromo(dimethyl sulfide)gold

Bromo[thiobis[methane]]gold, 9CI

[37922-40-0]

$BrAuSMe_2$

M 339.0
Useful starting material for synth. of Au(I) compounds. Air stable cryst. (C_6H_6/Me_2CO). Mp 130-140° dec.

Allen, E.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 2257 (*synth, ir*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1904 (*synth, ir*)
Roulet, R. *et al, Chimia*, 1975, **29**, 346.

$C_2H_6AuBr_3S$ IC-003157

Tribromo(dimethyl sulfide)gold

Tribromo[thiobis[methane]]gold, 9CI

[39929-04-9]

Br_3AuSMe_2

M 498.8
Yellow, air stable.

Ray, P.C. *et al, Indian J. Chem.*, 1930, **7**, 67 (*synth*)
Allen, E.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 2257 (*synth, ir*)

C_2H_6AuClS IC-003158

Chloro(dimethyl sulfide)gold(*I*)

Chloro[thiobis[methane]]gold, 10CI, 9CI

$ClAuSMe_2$

M 294.5
Useful starting material for synth. of Au(I) complexes. Air stable cryst. (C_6H_6/Me_2CO).

Ray, P.C. *et al, Indian J. Chem.*, 1930, **7**, 67 (*synth*)
Allen, E.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 2257 (*synth, ir*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1904 (*ir*)
Dash, K.C. *et al, Chem. Ber.*, 1973, **106**, 1221 (*synth, ir, nmr*)
Tamaki, A. *et al, J. Organomet. Chem.*, 1974, **64**, 411 (*synth*)
Roulet, R. *et al, Chimia*, 1975, **29**, 346 (*rev*)

$C_2H_6AuClSe$ IC-003159

Chloro(dimethyl selenide)gold(*I*)

Chloro[selenobis(methane)]gold, 9CI

[41867-97-4]

$ClAu(SeMe_2)$

M 341.4
Air stable. Cryst. (C_6H_6/Me_2CO). Mp 100° dec.

Dash, K.C. *et al, Chem. Ber.*, 1973, **106**, 1221 (*synth, nmr*)
Roulet, R. *et al, Chimia*, 1975, **29**, 346.

$C_2H_6AuCl_3S$ IC-003160

Trichloro(dimethyl sulfide)gold(*III*)

Trichloro[thiobis[methane]-S]gold, 9CI

[29826-91-3]

Cl_3AuSMe_2

M 365.4
Yellow, air-stable.

Ray, P.C. *et al, Indian J. Chem.*, 1930, **7**, 67 (*synth*)
Allen, E.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 2257 (*synth, ir*)

$C_2H_6AuS_2^{\ominus}$ IC-003161

Bis(methanethiolato)aurate(1−), 10CI

Bis(methylthio)aurate(1−)

$[MeSAuSMe]^{\ominus}$

M 291.1 (ion)

Tetrabutylammonium salt: [77424-98-7].
Colourless cryst. ($CHCl_3$/Et_2O). Mp 86-88°.

Bis(triphenylphosphine)iminium salt: [77679-34-6].
Colourless cryst. (aq. EtOH). Mp 188-189° dec.

Bowmaker, G.A. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 267 (*synth*)

$C_2H_6BBr_3S$ IC-003162

Tribromo(dimethyl sulfide)boron

Tribromo[thiobis[methane]]boron, 10CI. Thiobis[methane] compd. with tribromoborane (1:1), 9CI. Methyl sulfide compd. with boron bromide (BBr_3) (1:1), 8CI. Tribromoborane dimethyl sulfide

[29957-59-3]

$Me_2S—BBr_3$

M 312.6
Convenient means of handling the otherwise highly moisture-sensitive compd., BBr_3. White amorph. powder, stable to brief exp. to air or long-term storage under N_2. Mp 108°.

Schmidt, M., *et al, Chem. Ber.*, 1970, **103**, 3705 (*pmr*)
Peach, M.E., *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 75.
Bula, M.J. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1047 (*nmr, synth*)
Kinberger, K. *et al, Z. Naturforsch., B*, 1975, **30**, 55 (*synth*)
Brown, H.C. *et al, Inorg. Chem.*, 1977, **16**, 2938 (*synth, pmr*)
Williard, P.G. *et al, Tetrahedron Lett.*, 1980, **21**, 3731.

$C_2H_6BCl_2N$ IC-003163

Dichloro(dimethylamino)borane, 8CI

1,1-Dichloro-N,N-dimethylboranamine, 11CI, 10CI, 9CI. Dichloro(dimethylamino)borine

[1113-31-1]

Cl_2BNMe_2

M 125.7
Dimeric in solid state. Moisture sensitive, v. volatile liq., which slowly deposits cryst. of the dimer. Bp_{740} 11.5°, Bp_{35} 35°. ^{14}N nmr δ 297; ^{11}B nmr δ 30.8.

Dimer: [7392-25-8]. *Di-μ-chlorodichlorobis(dimethylamino) diborane*

$C_2H_6B_2Cl_4N_2$ M 251.5

Colourless cryst., stable to air and water. Mp 142°. ^{11}B nmr δ 10.4.

Bis-Py complex: [15590-29-1].

$C_{12}H_{16}BCl_2N_3$ M 283.9

White cryst. Subl.$_{0.1}$ 70°. Readily hydrol. in air.

Bis(4-methylpyridine) complex: [15590-34-8].

$C_{14}H_{20}BCl_2N_3$ M 312.0

White cryst. Mp 85°. Readily hydrol. in air.

Gunderloy, F.C. *et al, Inorg. Chem.*, 1962, **1**, 349.
Bannister, A.J. *et al, J. Chem. Soc.*, 1964, 995 (*synth, ir*)
Becher, H.J. *et al, Chem. Ber.*, 1965, **98**, 526 (*synth*)
Nöth, H. *et al, Chem. Ber.*, 1967, **100**, 3353; 1977, **110**, 2774; 1981, **114**, 1150 (*nmr, cmr, dimer*)
Lappert, M.F. *et al, J. Chem. Soc. A*, 1967, 602 (*synth, ir*)
King, G.H. *et al, Faraday Discuss. Chem. Soc.*, 1972, **54**, 70 (*pe*)
Fuss, W., *Z. Naturforsch., B*, 1974, **29**, 514 (*uv*)
Klusik, H. *et al, J. Organomet. Chem.*, 1982, **232**, C21.
Goumenard, J.P. *et al, Nouv. J. Chim.*, 1982, **6**, 143.

$C_2H_6BCl_3S$ IC-003164

Trichloro(dimethyl sulfide)boron

Trichloro[thiobis[methane]]boron, 10CI. Thiobis[methane] compd. with trichloroborane (1:1), 9CI. Methyl sulfide compd. with boron chloride (BCl_3) (1:1), 8CI. Trichloroborane dimethyl sulfide

[5523-19-3]

$Me_2S—BCl_3$

M 179.3
Convenient means of handling trichloroborane, which is otherwise much more volatile and moisture-sensitive. White solid, stable on brief exp. to air or long-term storage under N_2. Mp 86-87°. Mp 85-90°. Bp 181.9°.

Morris, H.L. *et al, Inorg. Chem.*, 1966, **5**, 124.
Schmidt, M. *et al, Chem. Ber.*, 1970, **103**, 3705 (*pmr*)
Bula, M.J. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1047 (*nmr, synth*)
Brown, H.C. *et al, Inorg. Chem.*, 1977, **16**, 2938 (*synth, pmr*)
Williard, P.G. *et al, Tetrahedron Lett.*, 1980, **21**, 3731.
Glavincevski, B. *et al, Can. J. Chem.*, 1981, **59**, 3012 (*nmr*)

$C_2H_6BF_3O$ IC-003165

(Dimethyl ether)trifluoroboron

Trifluoro[oxybis[methane]]boron, 10CI. Oxybis[methane] compd. with trifluoroborane (1:1), 9CI. Methyl ether compd. with boron fluoride (BF_3) (1:1), 8CI. Trifluoroborane compd. with oxybis[methane] (1:1). Boron trifluoride dimethyl etherate. Trifluoroborane dimethyl ether

[353-42-4]

$Me_2O—BF_3$

M 113.8
Catalyst for epoxide reactions. Commercially available. Moisture-sensitive liq. d 1.239. Mp −14°. Bp 126-127°. n_D^{20} 1.3079.

▷ Corrosive, flammable. ED8400000.

Fratiello, A. *et al, J. Org. Chem.*, 1972, **37**, 2237 (*nmr*)
Derouault, J. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 359 (*raman, ir*)
Fratiello, A. *et al, J. Chem. Soc., Perkin Trans. 2*, 1975, 1415 (*cmr*)
Umeyama, H., *Chem. Pharm. Bull.*, 1980, **28**, 1633 (*struct*)
Hirota, F. *et al, J. Mol. Struct.*, 1981, **70**, 305 (*struct*)
Iijima, K. *et al, J. Mol. Struct.*, 1981, **77**, 271 (*ed*)
Achiba, Y. *et al, J. Phys. Chem.*, 1982, **86**, 681 (*pe*)
Frost, D.C. *et al, J. Phys. Chem.*, 1982, **86**, 1917 (*pe*)
Hunt, R.L. *et al, Spectrosc.: Int. J.*, 1982, **1**, 45 (*matrix, ir*)

IC-003166

C_2H_6BN

Borane isocyanomethane

Trihydro(isocyanomethane)boron, 10CI. Methyl isocyanide borane

[62630-46-0]

$MeNC{-}BH_3$

M 54.8

Dipole moment 6.73D.

Stevans, J.F. *et al, J. Am. Chem. Soc.*, 1977, **99**, 1442 (*struct, microwave, synth*)
Umeyama, H. *et al, Chem. Pharm. Bull.*, 1980, **28**, 2279.
Bevan, J.W. *et al, Spectrochim. Acta, Part A*, 1981, **37**, 601 (*pe*)
Watari, F., *Inorg. Chem.*, 1982, **21**, 1442 (*ir, raman*)

IC-003167

$C_2H_6BN_3$

Azidodimethylborane, 9CI

Dimethylboron azide

[7360-67-0]

$Me_2B{-}N_3$

M 82.9

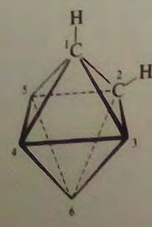
Paetzold, P.I. *et al, Z. Anorg. Allg. Chem.*, 1966, **345**, 79 (*synth, ir, pmr, B-11 nmr*)
Hauser-Wallis, R. *et al, Inorg. Chem.*, 1990, **29**, 3286 (*ed, struct*)

IC-003168

$C_2H_6B_4$

1,2-Dicarbahexaborane(6)

[20693-68-9]



M 73.3

closo-. Colourless liq. Isom. at 250° to 1,6-Dicarbahexaborane(6), IC-003169.

Shapiro, I. *et al, J. Am. Chem. Soc.*, 1963, **85**, 3167 (*synth, nmr, ms*)
Onak, T. *et al, Inorg. Chem.*, 1964, **3**, 1686 (*nmr*)
Beaudet, R. *et al, J. Chem. Phys.*, 1970, **53**, 1899 (*microwave*)

IC-003169

$C_2H_6B_4$

1,6-Dicarbahexaborane(6), 10CI

[20693-67-8]

M 73.3

closo-. Colourless liq. Mp −29.5° (−32.6°). Bp 22.7°.

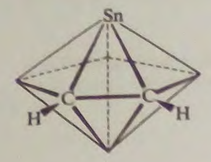
Shapiro, I. *et al, J. Am. Chem. Soc.*, 1963, **85**, 3167 (*synth, ir, nmr*)
Ditter, J. *et al, Inorg. Chem.*, 1970, **9**, 889 (*synth*)

IC-003170

$C_2H_6B_4Sn$

2,3-Dicarba-1-stannaheptaborane(6), 10CI

[63181-06-6]



M 192.0

closo-. Off-white solid. Sol. CH_2Cl_2. $Subl._{0.0001}$ 70-120° (cold finger).

Wong, K. *et al, Inorg. Chem.*, 1977, **16**, 2053 (*synth, ir, nmr, ms*)

IC-003171

$C_2H_6B_5F$

5-Fluoro-2,4-dicarbaheptaborane(7)

[55124-17-9]

M 103.1

closo-. Synth. from $[(Me)_3N][5\text{-Br-}2,4\text{-}C_2B_5H_6]$ + $[(C_4H_9)N]F$ in CH_2Cl_2. Ir ν 2620vs, 1410w, 1360vs, 1155s, 1050s, 880w, 690vw, 665vw cm^{-1}.

Marashin, N.J. *et al, Inorg. Chem.*, 1975, **14**, 1855 (*synth, ir, B-11 nmr*)
Ng, B. *et al, J. Fluorine Chem.*, 1985, **27**, 119 (*synth, ir*)
Durso, S.S. *et al, Inorg. Chem.*, 1989, **28**, 1615 (*microwave, gas phase struct, dipole moment*)

IC-003172

C_2H_6BrCuS

Bromo(dimethyl sulfide)copper(*I*)

Bromo[thiobis(methane)]copper, 9CI. Cuprous bromide methyl sulfide

[54678-23-8]

Me_2SCuBr

M 205.5

Cryst. deriv. for prepn. of organocuprate reagents. Prisms (Me_2S/hexane). Mp ca. 135° dec. Dissociates in soln.

House, H.O. *et al, J. Org. Chem.*, 1975, **40**, 1460 (*use*)
Posner, G., *Org. React. (N.Y.)*, 1975, **22**, 253 (*rev*)
San Filippo, J. *et al, Inorg. Chem.*, 1975, **14**, 1667 (*synth*)
Theis, A.B. *et al, Synth. Commun.*, 1981, **11**, 157 (*synth, use*)
Wuts, P.G.M., *Synth. Commun.*, 1981, **11**, 139 (*synth, use*)

IC-003173

$C_2H_6Br_4NO_2Re^{\ominus}$

Tetrabromo(ethanol)nitrosylrhenate(1−), 9CI

$[Re(NO)Br_4(EtOH)]^{\ominus}$

M 581.8 (ion)

Octahedral.

trans-form

Almost linear Re—N—O grouping with Re—N 172, N—O 119, Re—Br 250-253 pm. Ir ν_{NO} 1750-1735 cm^{-1}. Paramagnetic.

Et_4N salt: [56732-86-6].

Synth. by reaction of $(Et_4N)_2Re(NO)Br_5$ with EtOH. Green cryst. (EtOH). Dec. at 120-140°.

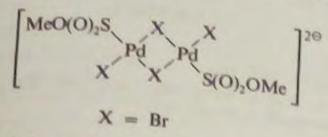
Ciani, G. *et al, Inorg. Chim. Acta*, 1975, **14**, L25 (*synth*)
Ciani, G. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 2156 (*cryst struct*)

$C_2H_6Br_4O_6Pd_2S_2^{2\ominus}$

IC-003174

Tetrabromobis(methylsulfonato)dipalladate(*II*)(2−)

Di-μ-bromodibromobis(methoxysulfonyl)dipalladate(II)(2−), 8CI



X = Br

M 722.6 (ion)

SO_3-trapped alkoxide intermed. in the oxidation of alcohols catalysed by $PdBr_2$.

Bis-Ph_4P salt: [58601-72-2].

Brown-orange solid. Sol. $CHCl_3$. Mp 190-192°.

Graziani, M. *et al, J. Organomet. Chem.*, 1971, **27**, C19 (*ir*)
Ros, R. *et al, Transition Met. Chem.*, 1975, **1**, 13 (*synth, ir, pmr*)

$C_2H_6CdCl_2N_2O_2$

IC-003175

Dichlorobis(formamide-*O*)cadmium

[32108-65-9]

$CdCl_2[O{=}C(NH_2)H]_2$

M 273.3

Polymeric struct. Prepd. from $CdCl_2$ + formaldehyde. Colourless prisms.

Nardelli, M. *et al, Ric. Sci.*, 1957, **27**, 2144; *CA*, **52**, 13510i (*synth*)
Mitschler, A. *et al, Acta Crystallogr.*, 1967, **22**, 236 (*cryst struct*)
Powell, D.P. *et al, Spectrochim. Acta, Part A*, 1985, **41**, 1023 (*ir, raman*)

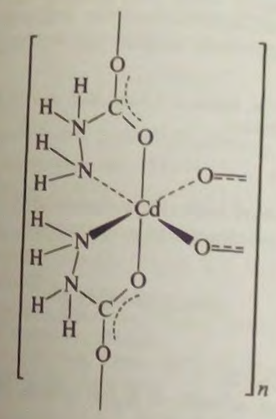
$C_2H_6CdN_4O_4$

IC-003176

Bis(carbazato)cadmium(*II*)

Bis(hydrazinecarboxylato-N′,O)cadmium(II)

[16404-33-4]



M 262.5

Distorted octahedral polymeric struct. Colourless cryst. (H_2O). Forms a monohydrate.

[11856-00-5]

Baibanti, A. *et al, Ric. Sci.*, 1966, **36**, 1210 (*synth*)

Baibanti, A. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1968, **126**, 307 (*cryst struct*)
Baibanti, A. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 100 (*cryst struct, hydrate, synth*)

$C_2H_6CdS_2$

IC-003177

Bis(methanethiolato)cadmium

Bis(methylthio)cadmium. Cadmium methanethiolate

[111317-14-7]

$Cd(SMe)_2$

M 206.6

Polymeric in solid state. Solid. Dec. at 260° to CdS and Me_2S.

Osakada, K. *et al, J. Chem. Soc., Chem. Commun.*, 1987, 1117 (*synth*)

$C_2H_6ClO_2Ti$

IC-003178

Chlorodimethoxytitanium(*III*), 11CI

[88092-83-5]

$TiCl(OMe)_2$

M 145.4

Synth. by reaction of $TiCl_3$ with excess trimethyl orthoformate. Light-brown solid. Mp 240° dec.

Giannetti, E. *et al, Inorg. Chim. Acta*, 1983, **74**, 215 (*synth, ir*)

$C_2H_6ClO_7S_2V$

IC-003179

Chlorobis(methylsulfonato-*O*)oxovanadium(*V*), 11CI

[90789-96-1]

$VOCl(OSO_2Me)_2$

M 292.5

Synth. by heating under reflux $VOCl_3$ and 2 moles $MeSO_3H$ in CCl_4. Orange-yellow solid. Ir $\nu_{V=O}$ 975 cm^{-1}.

Kumar, S. *et al, Indian J. Chem., Sect. A*, 1984, **23**, 200 (*synth, uv-vis, ir*)

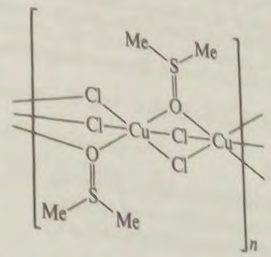
$C_2H_6Cl_2CuOS$

IC-003180

Dichloro(dimethyl sulfoxide)copper(*II*)

Dichloro[sulfinylbis[methane]-O]copper, 10CI. Copper(II) *chloride dimethylsulfoxide*

[72347-99-0]



M 212.5

Struct. comprises ferromagnetic linear chains of Cu ions with 3 bridging ligands between each pair. Coordination severely distorted from octahedral with 4 long and 2 short bonds. V. hygroscopic orange cryst. Sol. EtOH; insol. Et_2O. Mp 125° dec.

Selbin, J. *et al, J. Inorg. Nucl. Chem.*, 1961, **16**, 219 (*synth*)
Swank, D.W. *et al, Phys. Rev. B*, 1979, **20**, 2154 (*cryst struct*)

Landee, C.P. *et al*, *J. Appl. Phys.*, 1981, **52**, 2240 (*magnetism*)
Willett, R.D. *et al*, *J. Appl. Phys.*, 1982, **53**, 2677 (*esr*)
Satija, S.K. *et al*, *Phys. Rev. B*, 1982, **25**, 6855 (*nd*)

IC-003181

$C_2H_6Cl_2NOP$

Dimethylphosphoramidic dichloride, 9CI, 8CI
(Dimethylamino)phosphonic dichloride. Dimethylamino phosphoryl dichloride. Dichloro(dimethylamido) oxophosphorus(V)
[677-43-0]

$Me_2NP(O)Cl_2$

M 161.9
Liq. d_5^{25} 1.37. Bp 194-195°, Bp_{10} 76°, Bp_1 45°. n_D^{25} 1.4610.
▷ TB4025000.

Michaelis, A., *Justus Liebigs Ann. Chem.*, 1903, **326**, 129, 172 (*synth*)
Cowley, A.H. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 4454 (*pmr*)
Köttgen, D. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **385**, 56 (*ir, raman*)
Osokin, D.Ya. *et al*, *Org. Magn. Reson.*, 1972, **4**, 831 (*nqr*)
Robinson, E.A. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 1099 (*pmr, P-31 nmr*)
Gouesnard, J.P. *et al*, *Nouv. J. Chim.*, 1982, **6**, 143 (*N-15 nmr*)

IC-003182

$C_2H_6Cl_2NP$

Dimethylphosphoramidous dichloride, 9CI
Dichloro(dimethylamino)phosphine. Dichloro(dimethylamido) phosphorus(III)
[683-85-2]

Me_2NPCl_2

M 145.9
Ligand for Al, Fe, and Rh. Fuming liq. Bp 150°, Bp_{37} 56°. n_D^{20} 1.5020.
▷ V. reactive to oxidising agents. Reacts violently with H_2O and may inflame.

Burg, A.B. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 1107 (*synth*)
Nöth, H. *et al*, *Chem. Ber.*, 1961, **94**, 1505 (*synth*)
Durig, J.R. *et al*, *J. Phys. Chem.*, 1971, **75**, 3837 (*ir, raman*)
Biryukov, I.P. *et al*, *Zh. Obshch. Khim.*, 1972, **42**, 1223; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1972, **42**, 1217 (*nqr*)
Lappert, M.F. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1207 (*pe*)
Barlos, K. *et al*, *Z. Naturforsch., B*, 1978, **33**, 515 (*N-14 nmr*)
Gray, G.A. *et al*, *Org. Magn. Reson.*, 1980, **14**, 8 (*cmr*)
Duangthai, S. *et al*, *Org. Magn. Reson.*, 1982, **20**, 33 (*nmr, struct*)
Kukhar', V.P. *et al*, *Zh. Obshch. Khim.*, 1982, **52**, 562; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1982, **52**, 492 (*synth, P-31 nmr*)
Katsyuba, S.A. *et al*, *Zh. Obshch. Khim.*, 1984, **54**, 694; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1984, **54**, 615 (*ir, raman*)
Gloede, J., *Z. Anorg. Allg. Chem.*, 1985, **531**, 17 (*synth*)
Cavell, R.G. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1987, **43**, 215 (*pe*)
Kanjolia, R.K. *et al*, *Inorg. Chem.*, 1989, **28**, 3341 (*cmr, P-31 nmr*)

IC-003183

$C_2H_6Cl_2NPS$

Dimethylphosphoramidothioic dichloride, 9CI
(Dimethylamino)phosphonothioyl dichloride. Dichloro(dimethylamido)thiophosphorus(V)
[1498-65-3]

$Me_2NP(S)Cl_2$

M 178.0
Liq. d_4^{20} 1.377. Bp_{10} 75-76°. n_D^{20} 1.5404.

Godovikov, N.N. *et al*, *Zh. Obshch. Khim.*, 1961, **31**, 1628; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1961, **31**, 1516 (*synth*)
Keat, R. *et al*, *J. Chem. Soc. A*, 1968, 703 (*pmr*)
Köttgen, D. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **385**, 56 (*ir, raman*)
Osokin, D.Ya. *et al*, *Org. Magn. Reson.*, 1972, **4**, 831 (*nqr*)
Vilesov, F.I. *et al*, *Z. Phys. Chem.* (*Leipzig*), 1974, **255**, 661 (*pe*)
Shagidullin, R.R. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1975, **222**, 897; *Dokl. Phys. Chem.* (*Engl. Transl.*), 1975, **222**, 564 (*uv*)
Mathis, R. *et al*, *Spectrochim. Acta, Part A*, 1986, **42**, 519.

IC-003184

$C_2H_6Cl_2NSb$

Dichloro(dimethylamino)stibine
1,1-Dichloro-N,N-dimethylstibinamine, 11CI. Dichloro(dimethylamido)antimony
[95688-56-5]

Me_2NSbCl_2

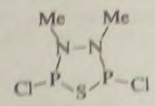
M 236.7
Solid. Mp *ca.* 180° dec.

Ensinger, U. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **514**, 137; 1985, **520**, 160 (*synth, ir, raman, ms*)

IC-003185

$C_2H_6Cl_2N_2P_2S$

2,5-Dichloro-3,4-dimethyl-1,3,4,2,5-thiadiazadiphospholidine, 9CI
[59725-20-1]



M 223.0
Liq.
▷ Reacts explosively with H_2O.

Nöth, H. *et al*, *Chem. Ber.*, 1976, **109**, 1942 (*synth, pmr, P-31 nmr, ms, props*)

IC-003186

$C_2H_6Cl_2NiOS$

Dichloro(dimethyl sulfoxide)nickel(*II*)
Dichloro(methylsulfoxide)nickel. Dichloro[sulfinylbis(methane)]nickel. Nickel(II) *chloride dimethyl sulfoxide complex*
[24597-20-4]

$NiCl_2(O{=}SMe_2)$

M 207.7
Probably octahedral struct. with bridging chlorides. Obtd. by heating $Ni(DMSO)_6Cl_2$ to110°. Yellow solid. Antiferromagnetically coupled. $\mu_{eff} = 2.91\mu_B$ (294K).
[27435-79-6]

Kanekar, C.R. *et al*, *Indian J. Chem., Sect. A*, 1970, **8**, 451 (*synth, uv-vis, ir, magnetism*)

IC-003187

$C_2H_6Cl_3OPdS^{\ominus}$

Trichloro(dimethyl sulfoxide)palladate(*II*)(1−)
Trichloro[sulfinylbis[methane]]palladate(1−)
[52573-98-5]

$[PdCl_3(O{=}SMe_2)]^{\ominus}$

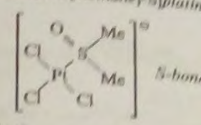
M 290.9 (ion)
K salt: [20647-43-2].
Obt. on cryst. of soln. of K_2PdCl_4 in aq. DMSO. Square garnet-red cryst. Sol. H_2O.

Kukushkin, Yu.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 835.
Kukushkin, Yu.N., *Zh. Prikl. Khim.* (*Leningrad*), 1968, **41**, 1407, 2381; *CA*, **69**, 80733; **71**, 56171 (*synth, ir, use*)

$C_2H_6Cl_3OPtS^{\ominus}$

IC-003188

Trichloro(dimethyl sulfoxide)platinate(*II*)(1−)
Trichloro(methyl sulfoxide)platinate(II)(*1−*), *8CI*
Trichloro[sulfinylbis[methane]-S]platinate(II)(*1−*), *9CI*



S-bonded-form

M 379.5 (ion)
Square planar struct.
O-bonded-form [33568-73-9]
K salt: [21350-35-6].
Probably does not exist.
S-bonded-form [31203-96-0]
Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + DMSO. Subject of mechanistic substitution studies.
K salt: [31168-86-2].
Bright orange solid. Sol. H_2O.
[33568-73-9, 51434-76-5, 60881-14-3]

Romeo, R. *et al*, *Inorg. Chem.*, 1974, **13**, 1991 (*synth, reactions*)
Melanson, R. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 1914 (*cryst struct*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 459 (*uv, Pt-195 nmr*)

IC-003189

$C_2H_6Cl_3PdS^{\ominus}$

Trichloro(dimethyl sulfide)palladate(*II*)(1−)
Trichloro[thiobis(methane)]palladate(1−), 11CI

$[PdCl_3(SMe_2)]^{\ominus}$

M 274.9 (ion)
Tetrapropylammonium salt: [84001-19-4].
Light brown cryst. (CH_2Cl_2/Et_2O). Mp 102-103°.

Goodfellow, R.J. *et al*, *J. Chem. Soc. A*, 1968, 504 (*synth, ir*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1904 (*synth, ir, raman*)
Guilliver, D.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1895 (*synth*)

IC-003190

$C_2H_6Cl_3PtS^{\ominus}$

Trichloro(dimethyl sulfide)platinate(*II*)(1−), 8CI
Trichloro[thiobis[methane]]platinate(II)(*1−*), *9CI*

$[PtCl_3(SMe_2)]^{\ominus}$

M 363.5 (ion)
Square planar. Synth. from $Pt_2Cl_4(SMe_2)_2 + Cl^{\ominus}$.
Tetrapropylammonium salt: [21194-12-7].
Orange-yellow needles (Me_2CO/Et_2O). Sol. CH_2Cl_2. Mp 117°.
Tetrabutylammonium salt: [59474-86-1].
Orange needles (Me_2CO/Et_2O). Sol. C_6H_6, CH_2Cl_2, EtOH, Me_2CO.

Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1904; 1976, 459 (*synth, ir, pmr, Pt-195 nmr*)
Kennedy, B.P. *et al*, *Inorg. Chem.*, 1977, **16**, 1744 (*reactions*)
Inorg. Synth., 1983, **22**, 128 (*synth*)

IC-003191

$C_2H_4Cl_4O_4Pd_2S_2^{2\ominus}$

Tetrachlorobis(methylsulfonato)dipalladate(*II*)(2−)
Di-μ-chlorodichlorobis(methoxysulfonyl)dipalladate(II)(*2−*), *8CI*
[31319-68-3]

As Tetrabromobis(methylsulfonato)dipalladate(*II*)(2−), IC-003174 with
X = Cl
M 544.8 (ion)
SO_3-trapped alkoxide reagent, in the oxidation of alcohols catalysed by $PdCl_2$.
Bis Ph_4P salt: [58548-27-7].
Orange solid. Sol. $CHCl_3$. Mp 175-179°.

Grenier, M. *et al*, *J. Organomet. Chem.*, 1971, **27**, C19 (*pr*)
Roa, R. *et al*, *Transition Met. Chem.*, 1975, **1**, 13 (*synth, ir, pmr*)

IC-003192

$C_2H_6Cl_5PdS^{\ominus}$

Pentachloro(dimethyl sulfide)palladate(*IV*)(1−)
Pentachloro[thiobis[methane]]palladate(1−), 11CI

$[PdCl_4(SMe_2)]^{\ominus}$

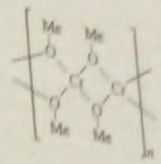
M 345.8 (ion)
Et_4N *salt:* [83971-13-9].
Orange solid. Sol. $PhNO_2$.

Guilliver, D.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1895 (*synth, ir, uv-vis*)

IC-003193

$C_3H_6CrO_2$

Chromium(*II*) methoxide
Dimethoxychromium. Chromium dimethoxide. Methanol chromium(2+) *salt*



M 114.0
Infinite chain struct. Synth. e.g. by methanolysis of chromocene in hydrocarbon solv. Violet, thermally stable, v. air-sensitive amorph. powder. Sl. sol. donor org. solvs. Reacts with halogenated solvs. to give air stable red-orange solns. Antiferromagnetic. No dec./subl. up to 250° under Ar.
▷ Oxidn. with excess dry O_2 can lead to violent explosions.

Votinsky, J. *et al*, *Collect. Czech. Chem. Commun.*, 1979, **44**, 88 (*synth, magnetism*)
Chisholm, M.H. *et al*, *Inorg. Chem.*, 1979, **18**, 120 (*synth*)
Horvath, B. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **457**, 51 (*synth, uv-vis*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 737 (*use*)

IC-003194

C_5H_5CuIS

Iodo(dimethyl sulfide)copper(*I*)
Iodo[thiobis[methane]]copper, 9CI
[54678-24-9]

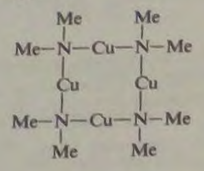
$ICuSMe_2$

M 252.5
Convenient precursor for the generation of lithium organocuprates. Cryst. (MeCN). Insol. most common org. solvs.

San Filippo, J. *et al*, *Inorg. Chem.*, 1975, **14**, 1667 (*synth*)
House, H.O., *J. Org. Chem.*, 1975, **40**, 1460 (*use*)
Mansson, J.E., *Acta Chem. Scand., Ser. B*, 1978, **32**, 543 (*synth, use*)

C_2H_6CuN IC-003195

Dimethylamidocopper(*I*)



tetramer

M 107.6
Tetrameric.
Tetramer: [111071-21-7]. *Tetrakis[μ-(N-methylmethanaminato)]tetracopper*
$C_8H_{24}Cu_4N_4$ M 430.4
V. thermally stable, v. air- and moisture-sensitive white cryst. Sol. THF, C_6H_6.

Gambarotta, S. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 1883 (*synth, pmr, cryst struct*)

$C_2H_6F_2NOP$ IC-003196

Dimethylphosphoramidic difluoride, 9CI
Dimethylamino phosphoryl difluoride.
Difluoro(dimethylamido)oxophosphorus(V)
[354-43-8]

$Me_2NP(O)F_2$

M 129.0
Liq. Bp_{12} 47-49°. n_D^{20} 1.4361.

Olah, G.A. *et al, Justus Liebigs Ann. Chem.*, 1959, **625**, 88 (*synth*)
Robinson, E.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 1099 (*pmr, P-31 nmr*)
Köttgen, D. *et al, Z. Phys. Chem.*, 1974, **92**, 289 (*ir, raman*)
Ryzhikov, B.D. *et al, Zh. Strukt. Khim.*, 1975, **16**, 754; *J. Struct. Chem. USSR* (*Engl. Transl.*), 1975, **16**, 700 (*F-19 nmr*)

$C_2H_6F_2NP$ IC-003197

Dimethylphosphoramidous difluoride, 9CI
Difluoro(dimethylamino)phosphine
[814-97-1]

Me_2NPF_2

M 113.0
Ligand for metals of groups VIB and VIII. Liq. d_4^{23} 1.10. Mp −87°. Bp_{704} 50°. n_D^{20} 1.3605. Readily oxidised.

Nöth, H. *et al, Chem. Ber.*, 1963, **96**, 1298 (*synth*)
Schmutzler, R., *Inorg. Chem.*, 1964, **3**, 415 (*ir, F-19, P-31 nmr*)
Morris, E.D. *et al, Inorg. Chem.*, 1969, **8**, 1673 (*cryst struct*)
Cradock, S. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 940 (*pe*)
Osokin, D.Ya. *et al, Org. Magn. Reson.*, 1972, **4**, 831 (*nqr*)
Forti, P. *et al, J. Am. Chem. Soc.*, 1973, **95**, 756 (*microwave, struct*)
Bach, M.-C. *et al, J. Mol. Struct.*, 1973, **17**, 23 (*struct*)
Lappert, M. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1207 (*pe*)
Barlos, K. *et al, Z. Naturforsch., B*, 1978, **33**, 515 (*N-14 nmr*)
Hill, W.E. *et al, Inorg. Chim. Acta*, 1979, **35**, 135 (*synth, complexes*)
Durig, J.R. *et al, J. Phys. Chem.*, 1989, **93**, 3041 (*microwave, ir, raman*)

$C_2H_6F_2NPS$ IC-003198

Dimethylphosphoramidothioic difluoride, 9CI, 8CI
(Dimethylamino)phosphonothioic difluoride.
Difluoro(dimethylamido)thiophosphorus(V)
[812-13-5]

$Me_2NP(S)F_2$

M 145.1
Liq. Bp_{30} 33-34°. n_D^{20} 1.4190.

Olah, G.A. *et al, Justus Liebigs Ann. Chem.*, 1959, **625**, 88 (*synth*)
Horn, H.-G. *et al, Z. Naturforsch., B*, 1966, **21**, 617, 729 (*pmr, F-19, P-31 nmr, ir*)
Reddy, G.S. *et al, Z. Naturforsch., B*, 1970, **25**, 1199 (*synth, pmr, P-31 nmr*)
Köttgen, D. *et al, Z. Phys. Chem. (Munich)*, 1974, **92**, 285 (*ir, raman*)
Yan, C.X. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1987, **42**, 49 (*pe*)
Cavell, R.G. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1987, **43**, 215 (*auger*)

$C_2H_6F_3IO_2$ IC-003199

Trifluorodimethoxyiodine
[53719-62-3]

$(MeO)_2IF_3$

M 245.9
Formed from IF_5 + $(MeO)_4Si$ in SO_2 at −30°. Yellow oil, slowly dec. at 0°.

Frohn, H.J. *et al, J. Fluorine Chem.*, 1984, **24**, 219 (*synth, F-19 nmr*)

$C_2H_6F_3NS$ IC-003200

(Dimethylamido)trifluorosulfur
DAST. Trifluoro(N-methylmethanaminato)sulfur, 9CI.
Dimethylaminosulfur trifluoride
[3880-03-3]

Me_2NSF_3

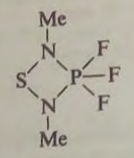
M 133.1
Fluorinating agent for alcohols, aldehydes, ketones etc. Liq. Mp −78.7°. Bp_{33} 49-49.5°.

▷ Explosive.

Demitras, G.C. *et al, Inorg. Chem.*, 1967, **6**, 1903 (*synth, ir, ms, F-19 nmr*)
Ibbott, D.G. *et al, Can. J. Chem.*, 1972, **50**, 2428 (*pmr, F-19 nmr*)
Middleton, W.J., *J. Org. Chem.*, 1975, **40**, 574 (*synth, F-19 nmr*)
Cochran, J., *Chem. Eng. News*, 1979, **57**, 4 (*haz*)
Middleton, W.J., *Chem. Eng. News*, 1979, **57**, 43 (*haz*)
Cowley, A.H. *et al, J. Am. Chem. Soc.*, 1979, **101**, 4074 (*pe*)
Heilmann, W. *et al, J. Fluorine Chem.*, 1988, **39**, 261 (*struct*)
Messina, P.A. *et al, J. Fluorine Chem.*, 1989, **42**, 137 (*haz*)

$C_2H_6F_3N_2PS$ IC-003201

3,3,3-Trifluoro-3,3-dihydro-2,4-dimethyl-1,2,4,3-thiadiazaphosphetidine, 8CI



M 178.1
1,1-Dioxide: [21465-17-8].
$C_2H_6F_3N_2O_2PS$ M 210.1

Synth. from PF_3Cl_2 + *N, N'*-dimethylsulfamide. Subl.$_{0.1}$ 50°.

Becke-Goehring, M. *et al, Z. Anorg. Allg. Chem.*, 1969, **365**, 185 (*synth, pmr, F-19, P-31 nmr*)

$C_2H_6F_5NO_2S_2$ IC-003202

(Dimethylimidosulfito-*N*)pentafluorosulfur
[80044-06-0]

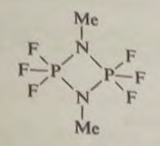
$(MeO)_2S{=}NSF_5$

M 235.1
Formed from $F_5SN{=}SF_2$ + NaOMe. Colourless liq. Vp <1 mm/25°.

Thrasher, J.S. *et al, J. Fluorine Chem.*, 1981, **18**, 537 (*synth, ir, ms, F-19 nmr, cmr*)

$C_2H_6F_6N_2P_2$ IC-003203

2,2,2,4,4,4-Hexafluoro-2,2,4,4-tetrahydro-1,3-dimethyl-1,3,2,4-diazadiphosphetidine
[3880-04-4]

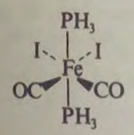


M 234.0
Synth. from PF_5 + $(Me_3Si)_2NMe$, or PF_5 + $MeNH_2/Me_3N$. Colourless liq. Mp −8.3° (−11°). Bp 89°. Reacts with nucleophilic agents, eg. alcohols, amines. $MeMgI/Et_2O$ replaces one F by Me; ^tBuLi replaces two F's. At 130° → $(MeN)_4P_3F_6^{\oplus}PF_6^{\ominus}$. HF → $[MeNH_3]PF_6$ + $(MeNHPF_4)_2$.

Yagupsky, M.P., *Inorg. Chem.*, 1967, **6**, 1770 (*ir, raman*)
Demitras, G.C. *et al, Inorg. Chem.*, 1967, **6**, 1903 (*synth*)
Almeningen, A. *et al, Acta Chem. Scand.*, 1969, **23**, 2179 (*ed, struct*)
Schmutzler, R., *J. Chem. Soc., Dalton Trans.*, 1973, 2687 (*synth, ir, pmr, F-19 nmr, P-31 nmr*)
Harris, R.K. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1912; 1976, 17, 306 (*reactions*)
Schlak, O. *et al, Org. Mass Spectrom.*, 1974, **9**, 582 (*ms*)
Haasemann, P. *et al, Z. Anorg. Allg. Chem.*, 1974, **408**, 293 (*synth, ir, raman*)
Charwath, M. *et al, Monatsh. Chem.*, 1977, **108**, 1093, 1359 (*reactions*)
Kubjacek, M. *et al, Monatsh. Chem.*, 1978, **109**, 587; 1981, **112**, 305, 1353 (*reactions*)
Meindl, W. *et al, Monatsh. Chem.*, 1979, **110**, 129, 135 (*reactions*)
Hahn, H. *et al, Monatsh. Chem.*, 1983, **114**, 1167; 1984, **115**, 881; 1985, **116**, 279 (*reactions*)
Kibrik, G.E. *et al, Magn. Reson. Chem.*, 1985, **23**, 903 (*F-19 nmr, struct*)
Utvary, K. *et al, Monatsh. Chem.*, 1986, **117**, 287, 1245 (*reactions*)
Galle, K. *et al, Monatsh. Chem.*, 1988, **119**, 53, 165 (*reactions*)

$C_2H_6FeI_2O_2P_2$ IC-003204

Dicarbonyldiiodobis(phosphine)iron, 9CI
[29845-14-5]



M 433.6

cis-form [35260-83-4]
Opaque brown cryst. (CH_2Cl_2).

Bigorgne, M. *et al, J. Organomet. Chem.*, 1970, **23**, 201 (*synth, spectra*)
Birck, J.L. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C.*, 1971, **273**, 880 (*cryst struct*)

$C_2H_6FeN_2O_2S_2^{\ominus}$ IC-003205

Bis(methanethiolato)dinitrosylferrate(1−)
$[Fe(NO)_2(SMe)_2]^{\ominus}$ (C_{2v})
[97773-69-8]

M 210.0 (ion)
Formed from diamagnetic dimer by reaction with nucleophile. Associated with cancerous states in animals. Paramagnetic.

Butler, A.R. *et al, Polyhedron*, 1985, **4**, 797 (*synth, esr*)

$C_2H_6FeO_6S_2$ IC-003206

Iron(*II*) methanesulfonate
Ferrous methanesulfonate. Bis(methanesulfonato)iron(II)
[56525-23-6]

$Fe[OS(O)_2Me]_2$

M 246.0
Hygroscopic grey-white powder. Sol. MeOH.

α-form

Synth. from $FeCl_2.4H_2O$ + $MeSO_3Ag$ in H_2O. Hygroscopic white solid. Remains paramagnetic down to 4.2K, but with some magnetic exchange.

β-form

Obt. from α-form on exposure to refluxing 2,2-dimethoxypropane for 3 days. White solid. Antiferromagnetic ordering occurs at 23K.

Methanesulfonic acid solvate:
$C_3H_{10}FeO_9S_3$ M 342.1
Synth. from $MeSO_3H$ + anhydrous $FeCl_2$ at 100°. White cryst.

▷ Synthetic route vigorous, evolving HCl (g).

Tetrakis-Py complex: see *Bis(methanesulfonato-O) tetrakis(pyridine)iron*(II), IC-011055

Haynes, J.S. *et al, Chem. Phys. Lett.*, 1980, **75**, 596 (*synth, mössbauer*)
Haynes, J.S. *et al, Can. J. Chem.*, 1981, **59**, 669; 1986, **64**, 744 (*synth, ir, magnetism, mössbauer*)

$C_2H_6Fe_2N_4O_4S_2$ IC-003207

Bis(μ-methanethiolato)tetranitrosyldiiron, 10CI
Bis(μ-methylthio)tetranitrosyldiiron. Roussin's red methyl ester. Roussin's red
[16071-96-8]

As Tetranitrosylbis(trifluoromethanethiolato)diiron, IC-002933 with

R = Me

M 325.9
Exists as an interconverting mixt. of *syn* and *anti* isomers in soln. Isol. from pickled vegetables. Reacts with secondary amines to give nitrosamines known to be carcinogenic. Fine red-brown or red-black needles (pentane). Mp 92-93° (88-89°). Ir ν_{NO} 1780vs, 1755vs cm^{-1} ($CHCl_3$).

▷ Carcinogenic.

[88643-17-8, 88643-72-5]

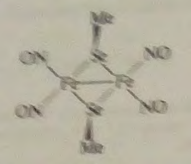
Li, M.-H. *et al, CA*, 1981, **94**, 25956, 133390, 18661 (*isol, tox*)

Bolt, W. *et al. Chem. Ber.*, 1981, **114**, 3194 (*synth, ir, pmr*)
Seyferth, D. *et al. Organometallics*, 1988, **5**, 539 (*synth, pmr, cmr, ir, ms*)
Gladwell, C. *et al. Polyhedron*, 1988, **7**, 1371 (*reactions, esr*)

$C_2H_6Fe_2N_2O_4Se_2$ IC-003208

Bis(μ-methaneselenolato)tetranitrosyldiiron, 11CI

[88716-15-5]



syn-form

M 419.7
Ir soln. exists as a mixt. of *syn* and *anti* isomers. Prep. from $Fe_2(CO)_6(\mu\text{-}SeMe)_2$ + NO. Vile-smelling red-purple cryst. (pentane). Mp 93-95°. Ir ν_{NO} 1778vs, 1747vs cm^{-1} ($CHCl_3$).

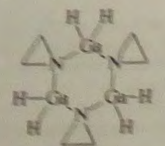
Butler, A.R. *et al. Inorg. Chem.*, 1985, **24**, 2851 (*nmr*)
Seyferth, D. *et al. Organometallics*, 1986, **5**, 539 (*synth, ir, pmr, cmr, ms*)

C_2H_6GaN IC-003209

1-Aziridinyldihydrogallium

1-Aziridylgallane

[34237-06-4]



trimer

M 113.7
Trimeric. Related compds. $(CH_2)_xNGaH_2$, x = 2-4 also descr.

Trimer: [34383-90-9]. *Tris[μ-(1-aziridinyl)] hexahydrotrigallium*, 9CI
$C_6H_{18}Ga_3N_3$ M 341.3
From aziridine + Me_3NGaH_3. Colourless air- and moisture-sensitive cryst. (by subl.).

Harrison, W. *et al. J. Chem. Soc., Chem. Commun.*, 1971, 1101 (*synth, cryst struct*)
Storr, A. *et al. J. Chem. Soc., Dalton Trans.*, 1972, 326 (*synth, pmr, ir, analyses*)
Harrison, W. *et al. J. Chem. Soc., Dalton Trans.*, 1972, 1554 (*cryst struct*)

$C_2H_6GeO_2$ IC-003210

(Acetyloxy)germane, 11CI

Germyl acetate. Acetatogermane

[58272-97-2]

H_3GeOAc

M 134.6
Synth. from GeH_3Br + AgOAc. Volatile liq. Mp 12.8°.

Srivastava, T.N. *et al. Can. J. Chem.*, 1962, **40**, 739; 1963, **41**, 1244 (*synth, ir*)

Angus, P.C. *et al. J. Chem. Soc., Dalton Trans.*, 1975, 2342 (*synth, pmr, ir, raman*)
Drake, J.E. *et al. Inorg. Nucl. Chem. Lett.*, 1976, **12**, 563 (*synth*)
Craddock, S. *et al. J. Organomet. Chem.*, 1985, **280**, 63 (*synth, ed*)

$C_2H_6HgS_2$ IC-003211

Bis(methylthio)mercury

Mercury methanethiolate. Bis(methanethiolato)mercury. Bis(methylmercapto)mercury

[21004-80-4]

$Hg(SMe)_2$

M 294.7
Monomeric in Py soln.; double chain struct. in solid state with dist. tetragonal pyramidal Hg (2 short Hg—S, 3 long Hg—S). Cryst. (EtOH or EtOH/EtOAc). Spar. sol. C_6H_6, cyclohexane; insol. H_2O. Mp 176-177°.

[6476-05-6]

Wertheim, E. *J. Am. Chem. Soc.*, 1929, **51**, 3661 (*synth*)
Bradley, B.C. *et al. J. Chem. Phys.*, 1964, **40**, 2258 (*cryst struct*)
Iwasaki, N. *et al. Bull. Chem. Soc. Jpn.*, 1974, **47**, 1323 (*raman, ir*)
Biscarini, P. *et al. J. Chem. Soc., Dalton Trans.*, 1974, 2140 (*ir, raman*)
Canty, A.J. *et al. Inorg. Chim. Acta*, 1976, **20**, 161 (*ir*)
Biscarini, P. *et al. Inorg. Chim. Acta*, 1981, **50**, 243 (*pe*)

C_2H_6LiN IC-003212

Lithium dimethylamide

N,N-Dimethylamine, lithium salt. LDA. N-Methylmethanamine, lithium salt, 9CI

[3585-33-9]

$LiNMe_2$

M 51.0
Commercially available. Strong base for org. chem.

▷ Pyrophoric; corrosive.

Goussnard, J.P. *et al. Nouv. J. Chim.*, 1982, **6**, 143 (*N-15 nmr*)

$C_2H_6MgO_2$ IC-003213

Magnesium methoxide

Dimethoxymagnesium. Methanol, magnesium salt, 8CI. Methyl alcohol, magnesium salt

[109-88-6]

$Mg(OMe)_2$

M 86.3
Prepd. by addn. of MeOH to a slurry of MgH_2 in C_6H_6. Alternatively, Mg can be dissolved in dry MeOH. Activators such as $HgCl_2$ can be used to promote reaction. Commercially available in MeOH soln. (8 wt. %). Catalyst for polym. of olefins. White solid. Moisture-sensitive. Reacts with H_2O to form $Mg(OH)_2$ and MeOH. Calcination in air or under vacuum yields, without hydrolysis, MgO. Sol. MeOH; insol. C_6H_6, THF.

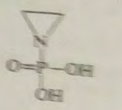
▷ Highly toxic.

U.K. Pat., 928 716, (1963); *CA*, **59**, 14022e (*manuf*)
Grigor'ev, A.I. *et al. Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **162**, 98; *CA*, **63**, 9239f (*ir*)
Ashby, E. *et al. Inorg. Chem.*, 1971, **10**, 906 (*synth, props*)
Hattori, T. *et al. J. Mater. Sci. Lett.*, 1983, **2**, 504 (*synth, calcination*)
Eur. Pat., 186 294, (1986); *CA*, **105**, 136473 (*synth*)

$C_2H_6NO_2P$

1-Aziridinylphosphinic acid, 9CI IC-003214

1-Aziridinophosphinic acid



M 123.0
Di-Me ester: [469-47-6]. *Dimethyl 1-aziridinylphosphonate*
$C_4H_{10}NO_3P$ M 151.1
Liq. d_4^{25} 1.215. Bp_{11} 126-128°, Bp_3 85-86°. n_D^{25} 1.4487.
Di-Et ester: [470-27-9]. *Diethyl 1-aziridinylphosphonate*
$C_6H_{14}NO_3P$ M 179.1
No phys. props. reported.
Di-Propyl ester: [42564-16-9]. *Dipropyl 1-aziridinylphosphonate*
Ovalbumin allergy suppressant in guinea pigs.
N,N,N',N'-Tetramethyldiamide: [1195-67-1]. *P-1-Aziridinyl-N,N,N',N'-tetramethylphosphonic diamide. 1-Aziridinylphosphonic bis(dimethylamide)*
$C_6H_{16}N_3OP$ M 177.1
Insect sterilant. Liq. d_4^{25} 1.07. Bp_1 96-97°, $Bp_{0.15}$ 42-46°. n_D^{25} 1.4680.
▷ TA 1/40000.

Sonnet, P.E. *et al. J. Org. Chem.*, 1966, **31**, 2982 (*amide, synth, pmr*)
Nifant'ev, E.E. *et al. Zh. Obshch. Khim.*, 1967, **37**, 1859; *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 1766 (*ester, amide, synth*)
Stagibilin, R.R. *et al. Zh. Obshch. Khim.*, 1968, **38**, 150; *J. Gen. Chem. USSR (Engl. Transl.)*, 1968, **38**, 148 (*ester, ir*)
Gray, G.A. *et al. J. Org. Chem.*, 1979, **44**, 1768 (*dimethyl ester, cmr, nmr*)
Dudykewitz, B. *et al. S. Afr. J. Chem.*, 1982, **35**, 63 (*dimethyl ester, synth, pmr*)
Dudykewitz, B. *et al. J. Chem. Soc., Perkin Trans. 2*, 1985, 303 (*reactions*)

$C_2H_6N_2S$ IC-003215

Carbamimidothioic acid methyl ester, 9CI

S-Methylisothiourea

[2986-19-8]

$HN{=}C(NH_2)SMe$

M 90.1
Free base not isol.
B.HCl: [53114-57-1].
Cryst. Mp 59-60°.
N-p-Toluenesulphonyl: Mp 118-119°.

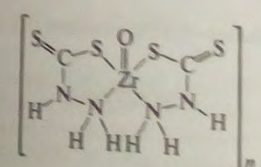
Taylor, J., *J. Chem. Soc.*, 1917, **111**, 655.
Org. Synth., Coll. Vol., 2, 1943, 411 (*synth*)

$C_2H_6N_4OS_4Zr$ IC-003216

Bis(hydrazinecarbodithioato-N^2,S^1)oxozirconium(*IV*), 11CI

Bis(dithiocarbazato)oxozirconium(IV)

[9585-06-9]



M 321.5

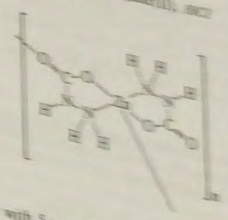
The syn- organic acetate appears a polymeric struct. Synth. from the acid and $ZrOCl_2$. Fungicidal. A_{50} = 1.44 μg_{Zr}
Agarwal, R.K. *et al. Curr. Sci.*, 1981, **50**, 406 (*synth, e, applications*)

$C_2H_6N_2O_2Zn$

Bis(methanaminato)zinc

Bis(dimethylamido)zinc. N-Dimethyl

[19486-23-3] IC-003217



M 215.4
Polymeric with 5-coord. zinc in solid state. Cryst. (H_2O).

[27114-36-9]

Frank, E. *et al. CA*, 1967, **67**, 3966 (*synth*)
Bigoli, F. *et al. Acta Crystallogr., Sect. B*, 1971, **27**, 305 (*cryst struct*)
Patil, K.C. *et al. J. Inorg. Nucl. Chem.*, 1979, **41**, 935 (*synth, e, thermal anal*)

$C_2H_6N_2O_2Zr$

Bis(hydrazinecarboxylato-N^1,O^2)oxozirconium(*IV*), 11CI IC-003218

[98776-42-2]

$(H_2NNHCOO)_2ZrO$

M 257.3
Synth. by passing CO_2 through an aq. soln. of $ZrOCl_2$, hydrazine and NaOH. White solid.

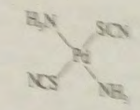
Agarwal, R.K. *et al. Orient. J. Chem.*, 1985, **1**, 65 (*synth, ir*)

$C_2H_6N_4PdS_2$

Diamminebis(thiocyanato-*S*)palladium(*II*) IC-003219

Diamminedithiocyanatopalladium(II)

[15660-25-0]



M 256.6
S-bonded struct. assigned on basis of ir spectrum. Cryst.

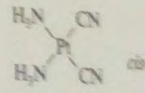
[75361-95-4, 75420-19-8]

Bleidelis, Ya.Ya. *et al. Kristallografiya*, 1957, **2**, 278, 287; *CA*, 1957, **51**, 14363, 14364 (*cryst struct*)
Turco, A. *et al. Nature (London)*, 1961, **191**, 66 (*synth, ir*)
Voityuk, A.A. *et al. Zh. Strukt. Khim.*, 1980, **21**, 20; *J. Struct. Chem. USSR (Engl. Transl.)*, 1980, **21**, 276 (*theory*)

$C_2H_6N_4Pt$

Diamminebis(cyano)platinum(*II*) IC-003220

[15020-95-8]



cis-form

M 281.1
Square planar. Configs. presumed from synthetic procedures.

cis-form [14523-27-4]
Synth. from Platinum(*II*) cyanide ($Pt(CN)_2$), IC-003474 + conc. aq. NH_3. White cryst. (hot conc. NH_3 soln.). Sol. H_2O. Ir ν_{CN} 2145, 2130 cm^{-1}.

trans-form [14095-76-2]
Synth. from *trans*-form of Diamminedichloroplatinum(*II*), IC-016643 + $CN^{\ominus}$. White needles. Sol. H_2O. Ir ν_{CN} 2130 cm^{-1}.

Kharitonov, Y.Y. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 248 (*ir*)
Isci, H. *et al*, *Inorg. Chem.*, 1975, **14**, 905 (*synth, uv, mcd*)

IC-003221

$C_2H_6N_4S_2$

1,2-Hydrazinedicarbothioamide, 9CI
2,5-Dithiobiurea, 8CI. Hydrazine-N,N′-bisthiocarbonamide. Hydrazidodicarbonthioamide. Dithiocarbamidohydrazine
[142-46-1]

$H_2NC(S)NHNHC(S)NH_2$

M 150.2
Needles (H_2O). Mp 214°, Mp 223° dec.
▷ EC1460000.

N-Benzoyl:
$C_9H_{10}N_4OS_2$ M 254.3
Cryst. (MeOH). Mp 257-259°.

N-Me: [34725-32-1].
$C_3H_8N_4S_2$ M 164.2
Cryst. (EtOH aq.). Mp 183-185°.

N-Benzyl: [66870-07-3].
$C_9H_{12}N_4S_2$ M 240.3
Powder. Mp 202-204°.

N,N′-Di Ph: [2209-59-8].
$C_{14}H_{14}N_4S_2$ M 302.4
Cryst. (EtOH). Mp 178-180°.

N,N,N′,N′-Tetra Me: [36340-47-3].
$C_6H_{14}N_4S_2$ M 206.3
Cryst. (Me_2CO). Mp 163°.

[26074-44-2]

Sadtler Standard Infrared Spectra, No. 12531.
Sadtler Standard NMR Spectra, No. 27654 (*pmr*)
Ohta, M. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1952, **72**, 1533 (*synth, uv*)
Klosa, J., *J. Prakt. Chem.*, 1958, **7**, 99 (*synth*)
Sugii, A. *et al*, *Yakugaku Zasshi* (*J. Pharm. Soc. Jpn.*), 1958, **78**, 306 (*N-Benzoyl*)
Mashima, M., *Bull. Chem. Soc. Jpn.*, 1964, **37**, 974 (*ir*)
Oliver, J.E. *et al*, *J. Med. Chem.*, 1972, **15**, 320 (*Tetra-Me*)
Furlani, C. *et al*, *Gazz. Chim. Ital.*, 1973, **103**, 951 (*N,N′-Di-Ph*)
Pignedoli, A. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1903 (*cryst struct*)
Williamson, K.L. *et al*, *Heterocycles*, 1978, **11**, 121 (*N-15 nmr*)
Altland, H.W. *et al*, *J. Heterocycl. Chem.*, 1978, **15**, 377 (*derivs*)
Indukumari, P.V. *et al*, *Indian J. Chem., Sect. B*, 1981, **20**, 387 (*derivs*)

IC-003222

$C_2H_6NiO_2$

Nickel(*II*) methoxide
Dimethoxynickel. Methanol, nickel(2+) salt (2:1)

$Ni(OMe)_2$

M 120.7
Probably contains 6-coord. Ni in polymeric struct. Pale green solid. Insol. org. solvs. μ_{eff} = 3.38μ_B.

Adams, R.W., *Aust. J. Chem.*, 1966, **19**, 207; 1967, **20**, 773 (*synth, magnetism, uv-vis, ir*)

IC-003223

$C_2H_6NiO_6$

Diaquabis(formato)nickel(*II*), 10CI
Nickel(II) *formate dihydrate*
[61633-69-0]

$Ni(OH_2)_2(O_2CH)_2$

M 184.7
Has polymeric struct. with octahedral Ni. Green solid.

Bircumshaw, L.L. *et al*, *J. Chem. Soc.*, 1950, 1800 (*synth*)
Korgmann, K. *et al*, *Z. Kristallogr.*, 1963, **118**, 291 (*cryst struct*)

IC-003224

$C_2H_6NiO_6S_2$

Bis(methanesulfonato)nickel(*II*)
Nickel(II) *methanesulfonate*

$Ni[OS(O)_2Me]_2$

M 248.8
Polymeric struct. with octahedral NiO_6. Synth. from $MeS(O)_2OH$ + $NiCl_2$ at 170° *in vacuo*. Yellow solid.

Paul, R.C. *et al*, *Indian J. Chem.*, 1974, **12**, 825 (*synth, ir, magnetism*)

IC-003225

$C_2H_6NiS_2$

Bis(methanethiolato)nickel(*II*)
Bis(methylmercapto)nickel(II). *Bis(methylthio)nickel. Nickel*(II) *methylmercaptide*

$Ni(SMe)_2$

M 152.8
Prob. 4-coordinate by analogy with Bis(ethanethiolato) nickel(*II*), IC-004171. Dark brown cryst. (Me_2CO/CH_2Cl_2). Sol. C_6H_6, Me_2CO. Reacts with CS_2 to afford $Ni(S_2CSMe)_2$.

Abel, E.W. *et al*, *J. Chem. Soc. A*, 1966, 1377 (*synth*)

IC-003226

$C_2H_6O_2Sn$

Tin(*II*) methoxide
Methanol, tin(2+) salt, 9CI
[14794-99-1]

$Sn(OMe)_2$

M 180.7
Synth. from $SnCl_2$ + Et_3N in MeOH. White ppt. Dec. without melting >100°. Easily hydrol. and oxidised.

Amberger, E. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1963, **2**, 395 (*synth*)
Morrison, J.S. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 393 (*synth, ir*)
Harrison, P.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 940 (*synth, mössbauer*)

IC-003227

$C_2H_6O_7S_2V$

Bis(methanesulfonato-*O*)oxovanadium(*IV*), 11CI
[90760-15-9]

$VO(OSO_2Me)_2$

M 257.1
Bis-Py complex: [90759-37-8].
$C_{12}H_{16}N_2O_7S_2V$ M 415.3

Synth. from Py and parent compd. Green solid. Paramagnetic; μ_{eff} = 1.78μ_B.
Tris-Py complex: [90759-39-0].
Blue solid. Paramagnetic; μ_{eff} = 1.75μ_B; Ir $\nu_{V=O}$ 1010 cm^{-1}.

Kumar, S. *et al*, *Indian J. Chem., Sect. A*, 1984, **23**, 200 (*derivs, synth, uv-vis, ir, magnetism*)

IC-003228

$C_2H_6O_{12}Zn_5$

Zinc carbonate hydroxide ($Zn_5(CO_3)_2(OH)_6$)
Bis(carbonato)hexahydroxypentazinc. Hydrozincate. Basic zinc carbonate
[12070-69-8]

$Zn_5(OH)_6(CO_3)_2$

M 549.0
Two Zn environments. 3 × Zn(1): octahedral, forms part of a sheet. 2 × Zn(2): tetrahedral, occurs above and below holes in sheets. 2 O of each CO_3 are bonded to an octahedral and a tetrahedral Zn, a 3rd O is H-bonded to 3 × OH groups. Synth. from ZnO, $(NH_4)_2CO_3$ and NH_3. Also formed by corrosion of Zn. Used in heat-developable photographic film; in deodorant compositions; in smoke inhibitors for pvc; in heat stabilisers for phenolic resins; fire-proofing agent; absorbant for H_2S; catalyst for cross-linking of epoxy coatings; oxidn. catalyst of amines; desulfurisation agent. Colourless cryst.

[5263-02-5, 39326-90-4, 66257-79-2]

Ghose, S., *Acta Crystallogr.*, 1964, **17**, 1051 (*cryst struct*)
Jambor, J.L. *et al*, *Can. Mineral.*, 1965, **8**, 385 (*powder struct*)
Hayek, E. *et al*, *Monatsh. Chem.*, 1966, **97**, 1059 (*synth, powder struct*)
Wiedemann, H.G., *Thermochim. Acta*, 1973, **7**, 131 (*thermal anal*)
Anulyunyan, G.A. *et al*, *Arm. Khim. Zh.*, 1984, **37**, 292 (*synth, ir*)

IC-003229

$C_2H_6PbS_2$

Bis(methanethiolato)lead
Bis(methylmercaptide. Bis(methylthio)lead. Lead(II) *methylmercaptide. Bis(methylthio)lead. Methanethiol lead(2+) salt, 9CI. Lead bis(methyl sulfide). Lead*(II) *methylthiolate*
[35029-96-0]

$Pb(SMe)_2$

M 301.4
Widely used intermediate, oxidised by air or I_2 to give disulfides or by HNO_3 to give thiosulfonic acid. Ppted. on addition of MeSH to aq. solns.of $Pb^{2\oplus}$ salts. Commercially available. Previously used as a sweetener in petrol. Moisture-sensitive yellow powder, dec. at 180-190° to give Me_2S and PbS.

Reid, E.E., *Organic Chemistry of Bivalent Sulphur*, Chemical Pub. Co., N.Y., 1958, **1**, 151 (*synth, uses*)

IC-003230

$C_2H_6PtS_2$

Bis(methanethiolato)platinum(*II*)
Bis(methylthio)platinum. Platinum(II) *methylmercaptide*

$Pt(SMe)_2$

M 289.2
Probably polymeric with square planar Pt. Formed by demethylation of SMe_2 or loss of SMe from other MeSR compds. Synth. from Platinum(*II*) chloride ($PtCl_2$), IC-016772 + SMe_2. Yellow solid.

Blomstrand, C.W., *J. Prakt. Chem.*, 1883, **27**, 161, 196 (*synth*)
Abel, E.W. *et al*, *J. Organomet. Chem.*, 1966, **5**, 260 (*synth*)

IC-003231

$C_2H_6S_2Zn$

Bis(methanethiolato)zinc
Zinc methanethiolate. Bis(methylthio)zinc. Bis(methylmercapto)zinc
[80813-48-5]

$Zn(SMe)_2$

M 159.5
Prob. polymeric. Source of β-ZnS on thermolysis at 260-280°. Solid. Insol. common org. solvs.

Firgo, H.A. *et al*, *J. Organomet. Chem.*, 1981, **222**, 201 (*synth, uses*)
Osakada, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1117 (*synth*)

IC-003232

$C_2H_7BCl_3N$

Trichloro(dimethylamine)boron
Trichloro(N-methylmethanamine)boron, 10CI. N-Methylmethanamine compd. with trichloroborane (1:1), 9CI. Dimethylamine boron trichloride. Dimethylamine trichloroborane. Trichloroborane dimethylamine
[13072-44-1]

$Me_2NH{-}BCl_3$

M 162.2
Fuming white solid or cryst. ($CHCl_3$), relatively stable to short air exp.

Kiesel, R. *et al*, *Inorg. Chem.*, 1973, **12**, 1090 (*ir*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*pmr*)
Ryschkewitsch, G.E. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1975, **5**, 123 (*synth*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1978, **17**, 1157 (*nmr*)
Haubold, W. *et al*, *Chem. Ber.*, 1980, **113**, 2333 (*synth*)

IC-003233

$C_2H_7BF_3N$

(Ethylamine)trifluoroboron
(Ethanamine)trifluoroboron, 10CI. Ethanamine compd. with trifluoroborane, 9CI. Ethylamine compd. with boron fluoride (BF_3) (1:1), 8CI. Boron trifluoride ethylamine. Trifluoroborane ethylamine
[75-23-0]

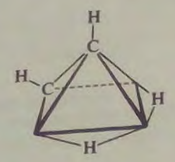
$EtNH_2{-}BF_3$

M 112.8
Widely used as a catalyst in industrial processes. Cryst. Et_2O, dec. rapidly when heated in air above Mp. Sol. C_6H_6, sl. sol. Et_2O. Mp 75-76°, Mp 89°. Bp_1 147-148°.
▷ KQ8060000.

Kraus, C.A. *et al*, *J. Am. Chem. Soc.*, 1929, **51**, 2690 (*synth*)
Gallais, F. *et al*, *CA*, 1960, **54**, 16064d (*struct, mord*)
Spitsyn, V.I. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **160**, 1101 (*synth*)
Meek, D.W. *et al*, *Inorg. Chem.*, 1966, **5**, 445 (*nmr*)
Elter, G. *et al*, *J. Organomet. Chem.*, 1972, **36**, 257.
Barber, M. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1973, **69**, 551 (*pe*)

IC-003234

$C_2H_7B_3$
1,2-Dicarbapentaborane(7), 10CI
[26249-71-8]



M 63.5
nido-. Colourless liq. by vacuum fractionation. Polym. at 50°.
Franz, D. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 1438 (*synth, ir, nmr*)

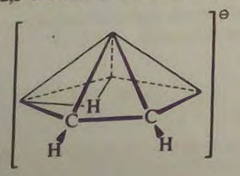
IC-003235

$C_2H_7B_3Si$
1-Silyl-1,5-dicarbapentaborane(5), 9CI
[55906-09-7]

M 91.5
Thompson, M.L. *et al*, *Inorg. Chem.*, 1972, **11**, 1925 (*ir*)
Leach, J.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1018 (*synth, nmr, ms*)

IC-003236

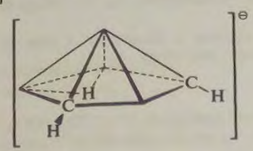
$C_2H_7B_4^{\ominus}$
Heptahydro-2,3-dicarbahexaborate(1 –), 10CI, 9CI



M 74.3 (ion)
nido-.
Li salt: [55927-70-3].
$C_2H_7B_4Li$ M 81.2
Sol. hexane, glyme, diglyme. Dec. at 160° in glyme.
Na salt: [38117-50-9].
$C_2H_7B_4Na$ M 97.3
Sol. diglyme, THF.
Onak, T. *et al*, *Inorg. Chem.*, 1966, **5**, 439 (*synth, ir, pmr, B-11 nmr*)
Onak, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2115 (*synth, pmr, B-11 nmr*)
Magee, K.P. *et al*, *J. Organomet. Chem.*, 1975, **86**, 159 (*synth*)

IC-003237

$C_2H_7B_4^{\ominus}$
Heptahydro-2,4-dicarbahexaborate(1 –)
[39394-97-3]



M 74.3 (ion)
nido-.
Li salt: Sol. MeCN.
Na salt: Sol. 1,2-dimethoxyethane.
Onak, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2115 (*synth, pmr, B-11 nmr*)
Abdou, Z.J. *et al*, *Inorg. Chem.*, 1988, **27**, 3679 (*synth, B-11 nmr*)

IC-003238

$C_2H_7B_5$
2,3-Dicarbaheptaborane(7), 11CI, 10CI, 9CI, 8CI
[30347-95-6]

M 85.1
closo-. Formed in v. low yield.
Rietz, R.R. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6254 (*synth, B-11 nmr, ms*)

IC-003239

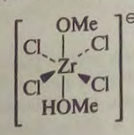
$C_2H_7B_5$
2,4-Dicarbaheptaborane(7), 10CI
[20693-69-0]
As μ-2,4-Dicarbaheptaborane(7)-2,4-diyldilithium, IC-003122 with

R = H

M 85.1
closo-. Parent compd. incorporated into high temp. polymers as silicon derivs. Colourless liq. by vacuum fractionation.
Beaudet, R. *et al*, *J. Chem. Phys.*, 1965, **43**, 2166 (*struct, microwave*)
Onak, T. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 4622 (*nmr, ir*)
Ditter, J. *et al*, *Inorg. Chem.*, 1968, **7**, 1748; 1970, **9**, 899 (*synth*)
Jotham, R. *et al*, *J. Chem. Soc. A*, 1971, 3181 (*ir, raman*)
Onak, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 76 (*ms*)
Onak, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 76 (*ms*)
Ditter, J. *et al*, *Inorg. Chem.*, 1976, **15**, 1063 (*nmr*)

IC-003240

$C_2H_7Cl_4O_2Zr^{\ominus}$
Tetrachloro(methanol)methoxyzirconate(*IV*)(1 –), 11CI
Tetrachloro(methoxy)methanolzirconate(IV)(*1* –)



M 296.1 (ion)
Me_3NH salt + Me_3NHCl: [106616-61-9].

Synth. fron $ZrCl_4(NMe_2)_2$ and boiling MeOH. Colourless solid (MeOH). Sol. MeOH. Mp 241-245° dec.
Karia, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 2493 (*cryst struct, synth*)

$C_2H_7N_2O_6Ru^{\ominus}$
(Glycinato-*N,O*)trihydroxy(nitrosyl)ruthenate(1 –) IC-003241
$[Ru(NO)(OH)_3(NH_2CH_2COO)]^{\ominus}$

M 256.1 (ion)
Detailed struct. unknown. Prepd. by treating Ru(NO)$Cl_3(OH_2)_2$ with glycine.
K salt: [67507-85-1].
Diamagnetic cryst. Sol. H_2O. Ir ν_{NO} 1865 cm^{-1}.
Ishiyama, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 619 (*synth*)
Honda, Y. *et al*, *CA*, 1981, **94**, 197304 (*synth*)

$C_2H_7OPSe_3$
***O*-Ethyl phosphorotriselenoate, 8CI** IC-003242
O-Ethyl triselenophosphate. O-Ethyl hydrogen phosphorotriselenoate. O-Ethyl phosphorotriselenoic acid. Ethoxobis(hydrogenselenido)selenophosphorus(V)

$EtOP(Se)(SeH)_2$

M 314.9
Unstable acid, isol. as di-K salt.
Di-K salt: [37443-16-6].
Solid. Mp 82°.
Gorak, R.D. *et al*, *Zh. Obshch. Khim.*, 1972, **42**, 56; *J. Gen. Chem. USSR (Engl. Transl.)*, 1972, **42**, 52.

$C_2H_7O_2P$
Ethyl phosphinate, 9CI IC-003243
Ethyl hypophosphite. Ethoxodihydridooxophosphorus(V). *Ethoxohydridohydroxophosphorus*(III)
[14684-32-3]

$EtOP(O)H_2 \rightleftharpoons EtOP(OH)H$

M 94.0
Liq. which cryst. at −20°. d_4^{20} 1.11. Bp_2 31-32°. n_D^{20} 1.4250. Dec. rapidly at r.t. giving yellow solid; stable only at <0° in inert atm. Oxid. in air. Stabilised by trace of EtOH.
▷ Spont. flammable.
Kabachnik, M.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1960, 146; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1960, 138 (*synth, props*)
Fitch, S.J., *J. Am. Chem. Soc.*, 1964, **86**, 61 (*synth, pmr, P-31 nmr*)
Pinnick, H.W. *et al*, *Synth. Commun.*, 1979, **9**, 535 (*synth, pmr, cmr, P-31 nmr, ir, props*)

$C_2H_7O_3P$ IC-003244
Monoethyl phosphonate, 9CI
Monoethyl phosphite. Ethoxohydridohydroxooxophosphorus(V). *Ethoxodi(hydroxo)phosphorus*(III)
[15845-66-6]

$EtOPH(O)OH \rightleftharpoons EtOP(OH)_2$

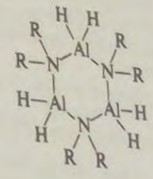
M 110.0
Tautomeric. Thermally unstable liq. pK_a 0.9 (est.). n_D^{20} 1.4230 (undist.).
Na salt: [39148-16-8].
Needles (EtOH). Mp 183°.
Al salt: [39148-24-8]. *Fosetyl, BSI. Phosethyl AL. LS 74 783. Aliette*
Fungicide having widespread use against zoospores and sporangics, but not mycelial growths.
p-Chlorobenzylisothiouronium salt: Solid. Mp 140-142°.
NH_4 salt: Cryst. (EtOH/Me_2CO). Mp 99-100°.
Michalski, J. *et al*, *J. Chem. Soc.*, 1961, 4905 (*synth*)
Hammond, P.R., *J. Chem. Soc.*, 1962, 2521 (*synth*)
Zwierzak, A. *et al*, *Tetrahedron*, 1973, **29**, 1089 (*synth*)
Kluba, M. *et al*, *Synthesis*, 1978, 134 (*synth, salts, ir, pmr*)
Davis, R.M., *Plant. Dis.*, 1982, **66**, 218 (*use*)
Kardanov, N.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1983, **268**, 364 (*P-31 nmr*)
Pesticide Manual, 7th Ed., 1983, 294.

$C_2H_7O_5PZn$
Aqua[monoethylphosphato(2 –)-*O*]zinc IC-003245
Zinc ethyl phosphate hydrate
[120313-05-5]

M 207.4 $Zn[P(O)_2OEt](OH_2)$
Phosphate groups form layers with tetrahedral zinc undulating perpendicular to the layer direction. Needles + $1H_2O$ (H_2O).
Ortiz-Avila, Y. *et al*, *Inorg. Chem.*, 1989, **28**, 2137 (*synth, cryst struct*)

$C_2H_8AgN_2^{\oplus}$
(Ethylenediamine)silver(*I*)(1+) IC-003246
(1,2-Ethanediamine-N,N')silver(1+), 10CI
$(H_2NCH_2CH_2NH_2)Ag^{\oplus}$
M 167.9 (ion)
Infinite chains in solid state with linear Ag. May exist as a hydrated chelate with 5 membered chelate ring in soln.
Nitrate: [77593-63-6].
$C_2H_8AgN_3O_3$ M 229.9
White cryst. Insol. cold H_2O.
Perchlorate: [71202-28-3].
White solid.
▷ Potentially explosive.
[68949-47-3]
Bang, E. *et al*, *Acta Chem. Scand., Ser. A*, 1978, **32**, 555 (*cryst struct*)
Bjerrum, J. *et al*, *Acta Chem. Scand., Ser. A*, 1979, **33**, 297 (*synth, props*)

C_2H_8AlN
(Dimethylamido)dihydroaluminium IC-003247
Dimethylaminoalane
[865-45-2]



Trimer

R = Me

M 73.0

Trimeric. Catalyst for polym. of alkenes and propylene oxide. Reagent for conversion of esters to amides or nitriles.

Trimer: [19567-31-8]. *Hexahydrotris[μ-(N-methylmethanaminato)]trialuminium, 9CI*

$C_6H_{24}Al_3N_3$ M 219.2

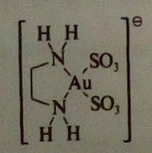
From AlH_3/Et_2O and Me_2NH or from $[Me_2NH_2]Cl$ and $LiAlH_4$. Colourless air and moisture sensitive cryst. (by subl.). Sol. Et_2O, C_6H_6. Mp 89-90°, 93-94°. $Bp_{0.01}$ 40-60°.

Wiberg, E. *et al, Z. Naturforsch., B*, 1955, **10**, 234 (*synth*)
Ruff, J.K. *et al, J. Am. Chem. Soc.*, 1961, **83**, 2836 (*synth, reactions*)
Marconi, W., *Eur. Polym. J.*, 1969, **5**, 747 (*use*)
Cesca, S. *et al, J. Polym. Sci., Part B*, 1969, **7**, 547 (*use*)
Ehrlich, R., *Inorg. Chem.*, 1970, **9**, 146 (*synth, reactions*)
Kovar, R.A. *et al, Inorg. Chem.*, 1971, **10**, 893 (*synth, pmr*)
Semenenko, K.N. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1972, **13**, 696 (*cryst struct*)
Basha, A. *et al, Tetrahedron Lett.*, 1977, 4171 (*use*)
Wood, J.L. *et al, Tetrahedron Lett.*, 1979, 4907 (*use*)

$C_2H_8AuN_2O_6S_2^{\ominus}$ IC-003248

(Ethylenediamine)disulfitoaurate(*III*)

(1,2-Ethanediamine-N,N')bis(sulfito)aurate(1−), 9CI



M 417.1 (ion)

Na salt: [52418-59-4].
Flaky cryst.

K salt: [52418-63-0].
Flaky cryst.

Ethylenediammonium(1+) salt: [52418-62-9].
Used in electrodeposition of gold. Colourless prisms (H_2O). Dec. slowly, forming metallic gold.

[52418-60-7, 55404-79-0]

U.S. Pat., 3 787 463, (1974); *CA*, **80**, 90408t (*synth, use*)
Dunand, A. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 370 (*cryst struct*)

C_2H_8BBrS IC-003249

Bromo(dimethyl sulfide)dihydroboron

Bromodihydro[thiobis[methane]]boron, 10CI. Bromoborane compd. with thiobis[methane] (1:1), 9CI. Bromoborane dimethyl sulfide

[55652-52-3]

$Me_2S—BH_2Br$

M 154.8

V. useful, stable reagent for selective hydroborations and prepn. of dialkylbromoboranes. Clear liq., sensitive to moisture. Sol. many aprotic solvs., particularly ethers and chlorinated hydrocarbons.

Kinberger, K. *et al, Z. Naturforsch., B*, 1975, **30**, 55 (*synth*)
Brown, H.C. *et al, Synthesis*, 1977, 695 (*synth*)
Wisian-Neilson, P. *et al, J. Inorg. Nucl. Chem.*, 1979, **41**, 1545 (*synth*)
Foret, C.J. *et al, J. Inorg. Nucl. Chem.*, 1979, **41**, 1661 (*synth*)
Brown, H.C. *et al, J. Org. Chem.*, 1979, **44**, 2417, 2422.

C_2H_8BClS IC-003250

Chloro(dimethyl sulfide)dihydroboron

Chlorodihydro[thiobis(methane)]boron, 10CI. Chloroborane compd. with thiobis(methane) (1:1). Chloroborane dimethyl sulfide

[63348-81-2]

$Me_2S—BH_2Cl$

M 110.4

A useful source for prepn. of dialkylchloroboranes and dialkyl(hydroxy)boranes. Colourless viscous liq., indefinite stability at r.t. in the absence of moisture; hydrol. by H_2O. As usually prepared, contains a few per cent of BH_3SMe_2 and $BHCl_2SMe_2$.

Brown, H.C. *et al, Inorg. Chem.*, 1977, **16**, 2938 (*synth, pmr, nmr*)
Brown, H.C. *et al, J. Org. Chem.*, 1977, **42**, 2533 (*synth*)
Kulkarni, S.V. *et al, J. Org. Chem.*, 1979, **44**, 1747.
Brown, H.C. *et al, J. Org. Chem.*, 1979, **44**, 2417, 2422; 1980, **45**, 4540.
Paget, W.E. *et al, J. Chem. Soc., Chem. Commun.*, 1980, 1169 (*synth*)

C_2H_8BIS IC-003251

(Dimethyl sulfide)dihydroiodoboron

Dihydroiodo[thiobis[methane]]boron, 10CI. Iodoborane complex with thiobis[methane], 9CI. Iodoborane methyl sulfide. Iodoborane dimethyl sulfide. MIBS

[55652-50-1]

$Me_2S—BH_2I$

M 201.8

Synth. from borane dimethylsulfide, iodine and triiodoborane. Useful hydroborating agent for the synth. of dialkyliodoboranes. Stable cryst., slowly hydrol. in moist air.

Kinberger, K. *et al, Z. Naturforsch., B*, 1975, **30**, 55 (*synth, nmr*)
Brown, H.C. *et al, J. Org. Chem.*, 1979, **44**, 2417, 2422 (*use*)

C_2H_8BN IC-003252

Aminodimethylborane, 8CI

1,1-Dimethylboranamine, 10CI, 9CI. Aminodimethylborine

[15973-91-8]

Me_2BNH_2

M 56.9

Air- and moisture-sensitive.

Dimer: [30442-90-1].
$C_4H_{16}B_2N_2$ M 113.8
Characterised spectroscopically.

Hoffmann, R., *J. Chem. Phys.*, 1964, **40**, 2474.
Nöth, H. *et al, Chem. Ber.*, 1967, **100**, 3353 (*dimer*)
Chakrabarty, M.R. *et al, Inorg. Chem.*, 1967, **6**, 518.
Nöth, H. *et al, J. Organomet. Chem.*, 1968, **12**, 23 (*pmr*)
Nöth, H. *et al, Chem. Ber.*, 1981, **114**, 1150 (*nmr*)

C_2H_8BN IC-003253

(Dimethylamino)borane, 8CI

N,N-Dimethylboranamine, 10CI, 9CI. (Dimethylamino)borine

[1838-13-7]

Me_2NBH_2

M 56.9

Dimeric at r.t., dissociates at higher temps. Reducing agent. Used in photographic development and nickel plating.

Dimer: [26085-03-0].
$C_4H_{16}B_2N_2$ M 113.8
Solid by subl. Mp 74.3-74.5°. V.p. 9.1mm at 23°.

Hoffmann, R., *J. Chem. Phys.*, 1964, **40**, 2474.
Nöth, H. *et al, Chem. Ber.*, 1967, **100**, 3353 (*nmr*)
Spielman, J.R., *J. Chem. Educ.*, 1970, **47**, 225 (*synth*)
Bock, H. *et al, Chem. Ber.*, 1971, **104**, 1687 (*pe*)
Burg, A.B., *Inorg. Chem.*, 1973, **12**, 1448.
Nöth, H. *et al, Inorg. Chem.*, 1982, **21**, 706 (*struct*)

C_2H_8BP IC-003254

(Dimethylphosphino)borane, 10CI, 9CI, 8CI

Boryldimethylphosphine, 9CI. (Dimethylphosphino)borine

[43625-73-6]

Me_2PBH_2

M 73.8

Prepd. by thermolysis of Me_2PH-BH_3. Unstable with respect to trimer, tetramer and not isol. in monomeric form.

Trimer:
$C_6H_{24}B_3P_3$ M 221.6
Sol. THF. Mp 86°. Bp 235° (est.).

Tetramer:
$C_8H_{32}B_4P_4$ M 295.4
Sol. THF. Mp 161°. Bp 310° (est.).

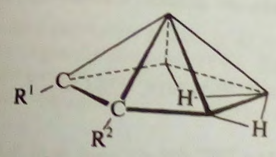
Homopolymer: [69773-26-8].
Used in electrophotographic plate insulating layers.

Burg, A.B. *et al, J. Am. Chem. Soc.*, 1953, **75**, 3872 (*synth*)
Florin, R.E. *et al, J. Am. Chem. Soc.*, 1954, **76**, 3344 (*ms*)
Hamilton, W.C. *et al, Acta Crystallogr.*, 1955, **8**, 199 (*struct*)
Burg, A.B. *et al, J. Inorg. Nucl. Chem.*, 1959, **11**, 258.
Wall, L.A. *et al, J. Res. Natl. Bur. Stand. (U.S.)*, 1959, **63**, 63 (*ms*)
Nöth, H. *et al, Z. Naturforsch., B*, 1960, **15**, 327 (*synth, use*)

$C_2H_8B_4$ IC-003255

2,3-Dicarbahexaborane(8)

[18972-20-8]



$R^1 = R^2 = H$

M 75.3

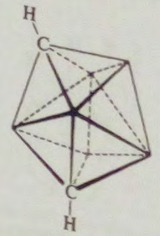
Colourless liq. Bp 56.9°.

Onak, T. *et al, J. Am. Chem. Soc.*, 1962, **84**, 2830 (*nmr*)
Streib, W. *et al, J. Am. Chem. Soc.*, 1963, **85**, 2331 (*struct*)
Onak, T. *et al, Inorg. Chem.*, 1966, **5**, 439 (*synth, ir, nmr*)

$C_2H_8B_6$ IC-003256

1,7-Dicarbaoctaborane(8), 10CI

[23732-90-3]



M 96.9

closo-. Sol. pentane. Mp 30°. Purif. by vacuum dist.

Garrett, P. *et al, Inorg. Chem.*, 1969, **8**, 1907 (*ir, nmr*)
Muetterties, E. *et al, Inorg. Chem.*, 1975, **14**, 950 (*nmr*)
Rogers, H. *et al, Inorg. Chem.*, 1976, **15**, 1775.

$C_2H_8Br_2CdN_4Se_2$ IC-003257

Dibromobis(selenourea-*Se*)cadmium(*II*), 9CI

Bis(selenourea)cadmium dibromide. Cadmium(II) bromide bis(selenourea)

[33702-45-3]

$[(H_2N)_2C{=}Se]_2CdBr_2$

M 518.2

Cryst.

Aitken, G.B. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2103 (*synth, ir*)

$C_2H_8Br_2N_4Se_2Zn$ IC-003258

Dibromobis(selenourea-*Se*)zinc

[38897-51-7]

$ZnBr_2[Se{=}C(NH_2)_2]_2$

M 471.2

Prepd. from $ZnBr_2$ + selenourea.

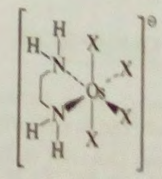
trans-form [34383-87-4]
Prepd. from $ZnSO_4$ + nicotinic acid. Colourless plates.

Aitken, G.B. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2103 (*synth, ir*)

$C_2H_8Br_4N_2Os^{\ominus}$ IC-003259

Tetrabromo(ethylenediamine)osmate(*III*)(1−), 9CI

Tetrabromo(1,2-diaminoethane)osmate(III)(1−)



X = Br

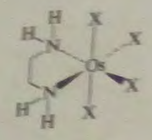
M 569.9 (ion)

Complexes of the type $[OsCl_nBr_{6-n}(en)]$ are also known.

Cs salt: [56148-16-4].
Obt. as a byproduct from the synth. of $OsBr_4$en. Yellow brown solid.

Bolourtschi, M.A. *et al, Z. Anorg. Allg. Chem.*, 1975, **415**, 25 (*synth, ir, uv, props*)

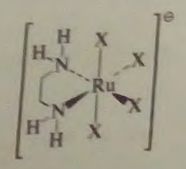
$C_2H_8Br_4N_2Os$ IC-003260
Tetrabromo(ethylenediamine)osmium(IV)
Tetrabromo(1,2-ethanediamine-N,N')osmium(IV), 9CI
[56148-12-0]



X = Br

M 569.9
Synth. from $K_2[OsBr_6]$ and anhydrous ethylenediamine. Dark green cryst. Related complexes also descr.
Bolourtschi, M.A. *et al, Z. Anorg. Allg. Chem.*, 1975, **415**, 25 (*synth, ir, uv, props*)

$C_2H_8Br_4N_2Ru^{\ominus}$ IC-003261
Tetrabromo(ethylenediamine)ruthenate(III)(1−)
Tetrabromo(1,2-ethanediamine-N,N')ruthenate(1−), 9CI
Tetrabromo(1,2-diaminoethane)ruthenate(III)(1−)
[15404-87-2]



X = Br

M 480.7 (ion)
Prepd. by treating (Ethylenediamine)bis(oxalato) ruthenate(III)(1−), IC-005025 with aq. HBr. Sol. H_2O.
Dibromobis(1,2-ethylenediamine)ruthenium(1+) salt: see *Dibromobis(ethylenediamine)ruthenium(III)(1+), IC-004332*
1,10-Phenanthrolinium(1+) salt: [17185-75-0].
Red-brown solid. Ir ν_{Ru-Br} 242, 205 cm^{-1}.
Broomhead, J.A. *et al, J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, magnetism*)

$C_2H_8CdCl_2N_4S_2$ IC-003262
Dichlorobis(thiourea-*S*)cadmium(*II*)
Bis(thiourea-S)cadmium dichloride. Cadmium(II) *chloride bis(thiourea)*
[15021-53-1]

$[(H_2N)_2C{=}S]_2CdCl_2$

M 335.5
Tetrahedral cadmium. Cryst. (aq. EtOH). Mp 210° dec. Dec. in dil. aq. soln. Dec. to CdS on heating.
Walter, G. *et al, Monatsh. Chem.*, 1934, **65**, 59 (*synth*)
Nardelli, M. *et al, Gazz. Chim. Ital.*, 1956, **86**, 1037; 1957, **87**, 137 (*cryst struct*)
Swaminathan, K. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 1291 (*ir*)
Flint, C.D. *et al, J. Chem. Soc. A*, 1966, 744 (*ir*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1967, 884 (*ir*)
Fridman, Ya.D. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 370 (*synth, stability const*)
Adams, D.M. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 631 (*synth, ir, raman*)
Krunks, M.J. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1985, **30**, 1373 (*thermal dec*)
Ashcroft, S.J. *et al, J. Chem. Eng. Data*, 1988, **33**, 73 (*heat of formn*)

$C_2H_8CdCl_2N_4Se_2$ IC-003263
Dichlorobis(selenourea-*Se*)cadmium(*II*), 9CI
Bis(selenourea)cadmium(II) *dichloride. Cadmium*(II) *chloride bis(selenourea)*
[23814-38-2]

$[(H_2N)_2C{=}Se]_2CdCl_2$

M 429.3
Isostructural with corresp. thiourea complex. Colourless cryst. (H_2O).
[38897-53-9]
Proskina, N.N. *et al, J. Struct. Chem. USSR* (*Engl. Transl.*), 1968, **9**, 983 (*synth, ir*)
Aitken, G.B. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2103 (*synth, ir*)

$C_2H_8CdI_2N_4O_2$ IC-003264
Diiodobis(urea-*O*)cadmium(*II*), 9CI
Bis(urea)cadmium diiodide. Cadmium(II) *iodide bis(urea)*
[14264-10-9]

$[(H_2N)_2C{=}O]_2CdI_2$

M 486.3
Cryst.
Belladen, L. *et al, Gazz. Chim. Ital.*, 1924, **54**, 568 (*synth*)
Durski, Z. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1975, **49**, 2101 (*powder struct*)
Santos, M.R.M.C. *et al, Thermochim. Acta*, 1988, **125**, 295 (*synth, ir, thermochem*)

$C_2H_8CdI_2N_4S_2$ IC-003265
Diiodobis(thiourea-*S*)cadmium(*II*), 9CI
Bis(thiourea)cadmium diiodide. Cadmium(II) *iodide bis(thiourea)*
[14240-52-9]

$[(H_2N)_2C{=}S]_2CdI_2$

M 518.4
Cryst. (H_2O). Mp 230° dec.
Flint, C.D. *et al, J. Chem. Soc. A*, 1966, 74 (*ir, synth*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1967, 884 (*ir*)
Durski, Z. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1975, **49**, 2101 (*powder struct*)
Ugai, Ya.A. *et al, Zh. Prikl. Khim.* (*Leningrad*), 1988, **61**, 2409 (*synth, ir*)

$C_2H_8CdN_4O_4$ IC-003266
(Ethylenediamine)dinitritocadmium
(1,2-Ethanediamine-N,N')bis(nitrito)cadmium, 9CI
[58220-77-2]

$Cd(NO_2)_2(NH_2CH_2CH_2NH_2)$

M 264.5
Heptahedral Cd in solid state in complex struct. with bridging NO_2 and ethylenediamine groups. Cryst.
[55926-76-6, 78379-69-8]
Shvelashvili, A.E. *et al, Koord. Khim.*, 1975, **1**, 467 (*cryst struct, ir*)
Kharitonov, Yu.Ya. *et al, Koord. Khim.*, 1981, **7**, 701 (*ir, raman*)

$C_2H_8CdN_6S_2$ IC-003267
Bis(hydrazine-*N*)bis(thiocyanato)cadmium
[34797-79-0]

$Cd(NH_2NH_2)_2(NCS)_2$

M 292.6
Colourless cryst. Spar. sol. H_2O. Dec. in hot H_2O to $Zn(OH)_2$.
Ray, P. *et al, J. Chem. Soc.*, 1920, **117**, 321 (*synth*)
Ferrari, A. *et al, Gazz. Chim. Ital.*, 1961, **91**, 69 (*struct*)
Aliev, R.Ya. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1972, **17**, 44 (*synth*)

$C_2H_9ClHgN_4S_2^{\oplus}$ IC-003268
Chlorobis(thiourea-*S*)mercury(1+)

$[(H_2N)_2C{=}S]_2HgCl^{\oplus}$

M 388.2 (ion)
Trigonal geometry.
Chloride: [29893-49-0]. *Dichlorobis(thiourea-S)mercury. Mercury*(II) *chloride bis(thiourea)*
$C_2H_8Cl_2HgN_4S_2$ M 423.7
Plates (H_2O). Mp 250° dec.
[15020-97-0]
Inorg. Synth., 1960, **6**, 26 (*synth*)
Swaminathan, K. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 1291 (*ir*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1967, 884 (*ir*)
Brotherton, P.D. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 334 (*synth, cryst struct*)
Marcotrigiano, G.O. *et al, Inorg. Chim. Acta*, 1974, **9**, 5 (*ir*)

$C_2H_8Cl_2CrN_4O_2$ IC-003269
Dichlorobis(urea-*O*)chromium(*II*), 10CI
Chromium(II) *chloride bis(urea)*
[67607-33-4]

$[CrCl_2[O{=}C(NH_2)_2]_2]_n$

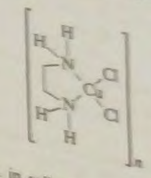
M 243.0
Chloride-bridged polymeric struct. Ir data indicates Cr—O coordn. Tetragonally distorted at Cr. Synth. from $CrCl_2.4H_2O$ and urea in EtOH. Pale blue air-sensitive cryst. Antiferromagnetic. μ_{eff} = 4.39μ_B (295K), 3.50μ_B (90K).
Larkworthy, L.F. *et al, Inorg. Chim. Acta*, 1978, **28**, 251 (*uv-vis, ir, magnetism, synth*)

$C_2H_8Cl_2CrN_4S_2$ IC-003270
Dichlorobis(thiourea-*S*)chromium(*II*), 10CI
[74624-12-7]

$[CrCl_2[S{=}C(NH_2)_2]_2]_n$

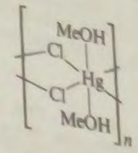
M 275.1
Polymeric chloride-bridged struct. with octahedral Cr. Yellow air-sensitive solid. μ_{eff} = 4.49μ_B (295K), 3.94μ_B (89K). Antiferromagnetic.
Larkworthy, L.F. *et al, Inorg. Chim. Acta*, 1980, **40**, 217 (*synth, uv, ir*)

$C_2H_8Cl_2CuN_2$ IC-003271
Dichloro(ethylenediamine)copper(*II*), 8CI
Dichloro(1,2-ethanediamine-N,N')copper(II), *8CI*
[22980-84-3]



M 194.5
Polymeric struct. in solid state with square planar Cu(en) Cl_2 units expanded to 6-coordination by bonding from Cu to two Cl atoms from adjacent units. Cryst. Insol. EtOH.
[39771-75-0]
Guseppetti, G. *et al, Rend. Soc. Mineral. Ital.*, 1965, **11**, 202 (*cryst struct*)
Billing, D.E. *et al, J. Chem. Soc. A*, 1969, 312 (*uv, esr, synth*)
Procter, I.M. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 3689 (*uv, esr, ir, synth*)
Frost, D.C. *et al, Mol. Phys.*, 1972, **24**, 861 (*pe*)
Reiff, W.M. *et al, Inorg. Chim. Acta*, 1978, **30**, 69 (*magnetism*)

$C_2H_8Cl_2HgO_2$ IC-003272
Dichlorobis(methanol)mercury(*II*)
Bis(methanol)mercury dichloride. Mercury(II) *chloride bis(methanol)*
[14875-34-4]



M 335.5
Polymeric chain struct. in solid state, as shown. Colourless cryst. (MeOH). Readily loses MeOH.
Madaule-Aubry, F., *Ann. Chim.* (*Paris*), 1965, **10**, 367 (*thermochem, heat of formn, props*)
Madaule-Aubrey, F., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **260**, 6613 (*cryst struct*)
Brusset, H. *et al, Bull. Soc. Chim. Fr.*, 1966, 3121 (*cryst struct*)

$C_2H_8Cl_2MnO_2$ IC-003273
Dichlorobis(methanol)manganese(*II*)
Manganese dichloride compd. with methanol (1:2)
[36301-49-2]

$MnCl_2(MeOH)_2$

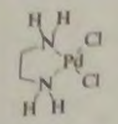
M 189.9
Struct. not known. Prepd. from $MnCl_2$ and anhyd. MeOH. Pink cryst. Forms $MnCl_2.MeOH$ at 85°. Compds. $MnCl_2.n$MeOH (n = 4, 3) also known.
Chkhenkeli, A.Z., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1957, **2**, 118 (*synth*)
l'Haridon, P. *et al, Rev. Chim. Minér.*, 1971, **8**, 813 (*synth, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, D1, 26 (*rev, bibl*)

$C_2H_8Cl_2N_2Pd$ IC-003274

Dichloro(ethylenediamine)palladium(*II*)

Dichloro(1,2-ethanediamine-N,N′)palladium, 9CI

[15020-99-2]



M 237.4

Square planar; isomorphous with Pt analogue. Orange-yellow needles. Sol. $CHCl_3$, CCl_4.

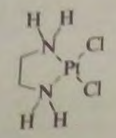
Drew, H.D.K. *et al, J. Chem. Soc.*, 1932, 1895 (*synth*)
Powell, D.B. *et al, Spectrochim. Acta*, 1961, **17**, 68 (*ir*)
Iball, J. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 1672 (*cryst struct*)

$C_2H_8Cl_2N_2Pt$ IC-003275

Dichloro(ethylenediamine)platinum(*II*), 8CI

Dichloro(1,2-ethanediamine-N,N′)platinum, 9CI

[14096-51-6]



M 326.0

Square planar struct. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + $NH_2CH_2CH_2NH_2$. Of special interest in reactions with biomolecules owing to neoplastic activity, but not used medicinally. Yellow cryst. Sol. H_2O.

▷ TP2497100.

Basolo, F. *et al, J. Am. Chem. Soc.*, 1950, **72**, 2433 (*synth*)
Berg, R.W. *et al, Spectrochim. Acta, Part A*, 1973, **29**, 319 (*ir*)
Iball, J. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 1672 (*cryst struct*)
Campbell, J.R. *et al, Inorg. Chem.*, 1978, **17**, 3622 (*raman*)
Nakayama, K. *et al, Bull. Chem. Soc. Jpn.*, 1984, **57**, 1336 (*uv, mcd*)
Butour, J.L. *et al, Biochem. Biophys. Res. Commun.*, 1985, **133**, 347 (*reactions*)

$C_2H_8Cl_2N_4O_2Pt$ IC-003276

Dichlorobis(urea-*N*)platinum(*II*)

$PtCl_2(NH_2CONH_2)_2$

M 386.0

Probably square planar struct. with *N*-bonded urea. Config. unknown. Yellow solid.

Drechsel, E., *J. Prakt. Chem.*, 1879, **20**, 469 (*synth*)
Penland, R.B. *et al, J. Am. Chem. Soc.*, 1957, **79**, 1575 (*ir*)

$C_2H_8Cl_2N_4S_2Te$ IC-003277

Dichlorobis(thiourea-*S*)tellurium(*II*), 9CI

Tellurium dichloride bis(thiourea)

[13930-98-8]

$[(H_2N)_2C{=}S]_2TeCl_2$

M 350.7

Synth. from $S{=}C(NH_2)_2$ + Na_2TeO_3 + NaCl. Yellow cryst., stable in air. Hydrol. by H_2O. Mp 184° dec.

Foss, O. *et al, Acta Chem. Scand.*, 1961, **15**, 1615 (*synth*)
Foss, O., *Acta Chem. Scand.*, 1962, **16**, 779 (*cryst struct*)
Hendra, P.J., *J. Chem. Soc. A*, 1967, 735 (*ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 11, 1978, **B3**, 139 (*bibl*)

$C_2H_8Cl_2N_4S_2Zn$ IC-003278

Dichlorobis(thiourea-*S*)zinc(*II*), 9CI

Bis(thiourea)zinc dichloride. Zinc(II) *chloride bis(thiourea)*

[14239-75-9]

$[(H_2N)_2C{=}S]_2ZnCl_2$

M 288.5

Tetrahedral Zn. Cryst. (H_2O). Mp 210° dec.

Naly, R., *Chem. Ber.*, 1876, **9**, 172 (*synth*)
Walter, G. *et al, Monatsh. Chem.*, 1934, **65**, 59.
Yamaguchi, A. *et al, J. Am. Chem. Soc.*, 1958, **80**, 527 (*synth, ir*)
Kuncher, N.R. *et al, J. Chem. Soc.*, 1958, 3478 (*cryst struct*)
Swaminathan, K. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 1291 (*ir*)
Flint, C.D. *et al, J. Chem. Soc. A*, 1966, 744 (*ir*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1967, 884 (*ir*)
Eaton, D.R. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 1007 (*pmr*)

$C_2H_8Cl_4HfN_4S_2$ IC-003279

Tetrachlorobis(thiourea-*S*)hafnium(*IV*), 11CI

Hafnium(IV) *chloride bis(thiourea)*

[84393-57-7]

$[(H_2N)_2C{=}S]_2HfCl_4$

M 472.5

See also Di-μ-chlorohexachlorobis(thiourea-*S*) dihafnium(*IV*), IC-003287. Struct. unknown. Thermochemical data suggest that the second thiourea molecule is not bonded to the hafnium.

Konunova, Ts.B. *et al, CA*, 1983, **98**, 60754g (*heat of formation*)
Konunova, Ts.B. *et al, Zh. Neorg. Khim.*, 1983, **28**, 788; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 447 (*synth, thermochem*)

$C_2H_8Cl_4N_2Os^{\ominus}$ IC-003280

Tetrachloro(ethylenediamine)osmate(*III*)(1−)

Tetrachloro(1,2-ethanediamine-N,N′)osmate(III)(*1−*), *9CI*

As Tetrabromo(ethylenediamine)osmate(*III*)(1−), IC-003259 with

X = Cl

M 392.1 (ion)

Obt. as a by-product from the synth. of $OsCl_4$(en).

Cs salt: [56148-15-3]. Dark brown.

Bolourtschi, M.A. *et al, Z. Anorg. Allg. Chem.*, 1975, **415**, 25 (*synth, ir, uv, props*)

$C_2H_8Cl_4N_2Os$ IC-003281

Tetrachloro(ethylenediamine)osmium(*IV*)

Tetrachloro(1,2-ethanediamine-N,N′)osmium(IV)

[56148-11-9]

As Tetrabromo(ethylenediamine)osmium(*IV*), IC-003260 with

X = Cl

M 392.1

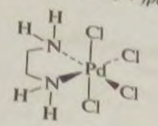
Synth. from $K_2[OsCl_6]$ and anhydrous ethylenediamine. Monoclinic red cryst.

Bolourtschi, M.A. *et al, Z. Anorg. Allg. Chem.*, 1975, **415**, 25 (*synth, ir, uv, props*)

$C_2H_8Cl_4N_2Pd$ IC-003282

Tetrachloro(ethylenediamine)palladium(*IV*)

Tetrachloro(1,2-ethanediamine-N,N′)palladium



M 308.3

Octahedral. Obtd. by chlorination of Dichloro(ethylenediamine)palladium(*II*), IC-003274 in CCl_4 or $CHCl_3$. Brown powder. Extended chlorination in aq. soln. yields $PdCl_6^{2\ominus}$.

Drew, H.D.K. *et al, J. Chem. Soc.*, 1932, 1895 (*synth*)
Kukushkin, Yu.N., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1963, **8**, 417 (*reaction*)

$C_2H_8Cl_4N_2Ru^{\ominus}$ IC-003283

Tetrachloro(ethylenediamine)ruthenate(*III*)(1−)

Tetrachloro(1,2-ethanediamine-N,N′)ruthenate(1−), 9CI.
Tetrachloro(1,2-diaminoethane)ruthenate(III)(*1−*)

[15404-86-1]

As Tetrabromo(ethylenediamine)ruthenate(*III*)(1−), IC-003261 with

X = Cl

M 302.9 (ion)

cis-Octahedral anion. Prepd. by treating (Ethylenediamine) bis(oxalato)ruthenate(*III*)(1−), IC-005025 with aq. HCl. Sol. H_2O.

Dichlorobis(1,2-ethylenediamine)ruthenium(*1+*) *salt:* see *Dichlorobis(ethylenediamine)ruthenium*(*1+*), *IC-004357*

1,10-Phenanthrolinium(*1+*) *salt:* [16960-80-8]. Orange solid. Ir ν_{RuCl} 330, 309, 285, 269 cm^{-1}.

Broomhead, J.A. *et al, J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, magnetism*)

$C_2H_8Cl_4N_4O_2Ti$ IC-003284

Tetrachlorobis(urea-*O*)titanium(*IV*), 11CI

Titanium(IV) *chloride bis(urea)*

[16924-10-0]

$[(H_2N)_2C{=}O]_2TiCl_4$

M 309.8

Synth. by adding excess $TiCl_4$ to a suspension of urea in CH_2Cl_2 and leaving for 5 days. Catalyses the cyclotrimerisation of butadiene. Yellow solid. Insol. CH_2Cl_2. Mp 215° dec.

Rivest, R. *et al, Can. J. Chem.*, 1962, **40**, 2234 (*synth, ir*)
Ionova, E.A. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1966, **11**, 74 (*synth*)
Kharitonov, Yu.Ya. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1966, **11**, 1284 (*ir*)
Japan. Pat., 68 13 451, (1968); *CA*, **70**, 77450z (*use*)

$C_2H_8Cl_4N_4S_2Ti$ IC-003285

Tetrachlorobis(thiourea-*S*)titanium(*IV*), 11CI

Titanium(IV) *chloride bis(thiourea)*

[84366-11-0]

$[(H_2N)_2C{=}S]_2TiCl_4$

M 341.9

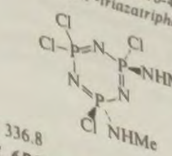
According to Rivest, ligand coordinates through nitrogen. Synth. by adding $TiCl_4$ to a suspension of thiourea in CH_2Cl_2. Dark brown solid. Mp 130° dec.

Rivest, R. *et al, Can. J. Chem.*, 1962, **40**, 2234 (*synth, ir*)
Konunova, Ts.B. *et al, CA*, 1983, **98**, 60754g (*thermochem*)

$C_3H_8Cl_4N_5P_3$ IC-003286

2,2,4,6-Tetrachloro-2,2,4,4,6,6-hexahydro-4,6-bis(methylamino)-1,3,5,2,4,6-triazatriphosphorine, 9CI

2,2,4,6-Tetrachloro-2,2,4,4,6,6-hexahydro-4,6-bis(methylamino)cyclotriphosphazene. 2,2,4,6-Tetrachloro-4,6-bis(methylamino)-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2,4,6-Tetrachloro-4,6-bis(methylamino)-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine



M 336.8 (*4RS,6RS*)-form

(*4RS, 6RS*)-*form* [16416-60-7]
trans-*form*
No phys. props. reported.

(*4RS, 6SR*)-*form* [16400-31-0]
cis-*form*
Cryst. (cyclohexane). Mp 145°.

Ray, S.K. *et al, J. Chem. Soc.*, 1961, 872 (*synth*)
Lehr, W., *Z. Anorg. Allg. Chem.*, 1967, **352**, 27 (*synth*)
Biran, Z. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1978, **8**, 185 (*synth, glc*)
Thomas, B. *et al, Z. Anorg. Allg. Chem.*, 1982, **489**, 131 (*N-14, P-31 nmr*)
Bamgboye, T.T. *et al, Spectrochim. Acta, Part A*, 1984, **40**, 329 (*pmr*)

$C_2H_8Cl_8Hf_2N_4S_2$ IC-003287

Di-μ-chlorohexachlorobis(thiourea-*S*)dihafnium(*IV*), 11CI

[84191-50-4]

$[(H_2N)_2C{=}S]_2Hf_2Cl_8$

M 792.8

Struct. not fully elucidated, but authors' proposal that only one thiourea is bonded to Hf is unlikely, cf Di-μ-chlorohexachlorobis(*N,N′*-diphenylthiourea-*S*) dihafnium(*IV*), IC-011853. Synth. from $HfCl_4$ and thiourea. White solid, unstable in moist air.

Monomer: [84366-12-1]. *Hafnium*(IV) *chloride thiourea. Tetrachloro(thiourea-S)hafnium*(IV), *11CI*

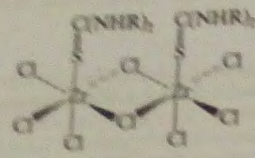
$CH_4Cl_4HfN_2S$ M 396.4

Konunova, Ts.B. *et al, CA*, 1983, **98**, 60754g (*heat of formn*)
Konunova, Ts.B. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 447, 515 (*synth, ir, thermochem*)

$C_2H_8Cl_8N_4S_2Zr_2$ IC-003288

Di-μ-chlorohexachlorobis(thiourea-*S*)dizirconium(*IV*), 11Cl

[84191-69-1]



R = H

M 618.3

Synth. by mixing ethyl acetate solns. of $ZrCl_4$ and thiourea. White solid, readily hydrol.

Monomer: [84366-13-2]. *Tetrachloro(thiourea)zirconium(IV). Zirconium tetrachloride thiourea. Zirconium(IV) chloride thiourea*

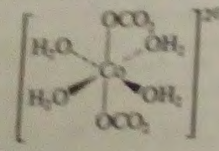
$CH_4Cl_4N_2SZr$ M 309.1

Not separately identified.

Kuznetsova, Ts.B. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 467, 515 (*synth, ir*)

$C_2H_8CoO_{10}^{2\ominus}$ IC-003289

Tetraaquabis(carbonato(2−)-*O*)cobaltate(2−), 9Cl



M 251.0 (ion)

trans-Octahedral at Co.

Di-K salt: [58592-59-9]. *Potassium cobalt carbonate tetrahydrate*

Rose-coloured cryst.

Reynolds, W.C. *et al., J. Chem. Soc.*, 1958, **73**, 262 (*synth*)

Harlow, R.L. *et al., Acta Crystallogr., Sect. B*, 1976, **32**, 466 (*cryst struct*)

$C_2H_8CrF_4N_2^{\ominus}$ IC-003290

(Ethylenediamine)tetrafluorochromate(*III*)(1−), 8Cl

(1,2-Ethanediamine-N,N′)tetrafluorochromate(III)(1−), 11Cl, 10Cl, 9Cl

M 188.0 (ion)

Octahedral complex.

cis-Bis(ethylenediamine)difluorochromium(III) salt: [13842-66-4]. *Bis(1,2-ethanediamine-N,N′)difluorochromium(1+) (1,2-ethanediamine-N,N′)tetrafluorochromate(1−)*

$C_4H_{16}Cr_2F_6N_8$ M 378.2

Starting material. Purple solid (aq. EtOH). Hydrol. rapidly in H_2O.

Ethylenediammonium(2+) salt, chloride: [94586-00-2]. Blue cryst.

[13521-43-4]

Vaughn, J.W. *et al., Inorg. Chem.*, 1973, **12**, 2346 (*synth*)

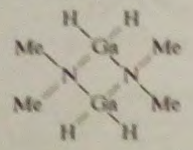
Diaz, C. *et al., Transition Met. Chem.*, 1984, **9**, 469 (*cryst struct, ir, uv-vis*)

Inorg. Synth., 1986, **24**, 185 (*synth, Cr(en)$_2$F$_2$ salt*)

C_2H_8GaN IC-003291

(Dimethylamido)dihydrogallium

Dimethylaminogallane



Dimer

M 115.8

Dimeric in gas phase and in C_6H_6; not monomeric as first reported. Synth. from Gallane, IC-019047 and Me_2NH.

Dimer: [97642-68-7]. *Tetrahydrobis[μ-(N-methylmethanaminato)]digallium, 11Cl. Bis[μ-(dimethylamido)]tetrahydrodigallium*

$C_4H_{16}Ga_2N_2$ M 231.6

White, air- and moisture-sensitive solid.

Greenwood, N.N. *et al., J. Chem. Soc. A*, 1966, 706 (*synth*)

Baxter, P.L. *et al., J. Chem. Soc., Dalton Trans.*, 1985, 807 (*synth, ed, ir, raman*)

$C_2H_8I_3N_3ORu$ IC-003292

(Ethylenediamine)triiodo(nitrosyl)ruthenium

(1,2-Ethanediamine-N,N′)triiodo(nitrosyl)ruthenium

$Ru(NO)I_3(NH_2CH_2CH_2NH_2)$

M 571.8

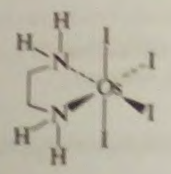
Reported in early literature; struct. unknown.

Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 225 (*synth*)

$C_2H_8I_4N_2Os$ IC-003293

(Ethylenediamine)tetraiodoosmium(*IV*)

[56148-13-1]



M 757.9

Synth. by reaction of Tetrachloro(ethylenediamine) osmium(*IV*), IC-003281 with HI. Dark blue cryst.

Bolourtchi, M.A. *et al., Z. Anorg. Allg. Chem.*, 1975, **415**, 25 (*synth, ir, uv*)

$C_2H_8I_4N_2Ru^{\ominus}$ IC-003294

(Ethylenediamine)tetraiodoruthenate(*III*)(1−)

(1,2-Ethanediamine-N,N′)tetraiodoruthenate(1−), 9Cl. (1,2-Diaminoethane)tetraiodoruthenate(III)(1−)

As Tetrabromo(ethylenediamine)ruthenate(*III*)(1−), IC-003261 with

X = I

M 668.7 (ion)

cis-Octahedral anion. Prepd. by treating (Ethylenediamine) bis(oxalato)ruthenate(*III*)(1−), IC-005025 with aq. HI. Sol. H_2O.

Bis(1,2-ethylenediamine)dichlororuthenium(1+) salt, 9Cl

Bis(ethylenediamine)dichlororuthenium(III)(1+), 8Cl: (004374

Broomhead, J.A. *et al., J. Chem. Soc. A*, 1967, 546 (*synth, str, ir, magnetism*)

$C_2H_8MnN_2O_4S_2$ IC-003295

Tetraaquabis(thiocyanato-*N*)manganese(*II*), 11Cl

Tetraaquabis(isothiocyanato)manganese(II). Manganese(II) isothiocyanate tetrahydrate

[93603-91-9]

$Mn(NCS)_2(OH_2)_4$

M 243.1

trans-Octahedral. Synth. from aq. solns. of $Ba(SCN)_2.2H_2O$ and $MnSO_4.4H_2O$. Pale green cryst. (H_2O). Mp 42°. Dehydration occurs at 135°, dec. of anhydrous salt at 432°. Struct. of 18-crown-6 adduct also determined.

Beagley, B. *et al., Inorg. Chim. Acta*, 1984, **89**, 163 (*synth, cryst struct, thermal props*)

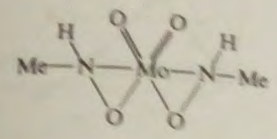
Zhang Wen-Xing, *et al., Acta Chim. Sin. (Engl. Ed.)*, 1987, **45**, 1143 (*cryst struct*)

$C_2H_8MoN_2O_4$ IC-003296

Bis(*N*-methylhydroxylamido)dioxomolybdenum(*VI*)

Bis(N-hydroxymethanaminato-N,O)dioxomolybdenum(VI), 11Cl, 10Cl

[70631-31-1]



M 220.0

Synth. from MoO_3 + $[MeH_2NOH]Cl$ in 2.5*M* KOH. Colourless cryst. (H_2O). Sol. H_2O, MeCN, DMF.

Wieghardt, K. *et al., Angew. Chem., Int. Ed. Engl.*, 1979, **18**, 548 (*cryst struct, synth*)

Wieghardt, K. *et al., Inorg. Chem.*, 1980, **19**, 2927 (*reactions, props*)

Minelli, M. *et al., Inorg. Chem.*, 1983, **22**, 3952 (*Mo-95 nmr*)

Hahn, M. *et al., Inorg. Chim. Acta*, 1984, **89**, L31 (*reactions*)

$C_2H_8NPS_3$ IC-003297

Dimethylphosphoramidotrithioic acid, 9Cl, 8Cl

(Dimethylamido)bis(hydrogensulfido)thiophosphorus(V)

$Me_2NP(S)(SH)_2$

M 173.2

Di-Ph ester: Diphenyl dimethylphosphoramidotrithioate

$C_{14}H_{16}NPS_3$ M 325.4

Visc. liq. $Bp_{0.05}$ 110°.

Fr. Pat., 1 378 035, (1964); *C.A.*, **62**, 10371.

$C_2H_8N_2Ni^{2\ominus}$ IC-003298

Ethylenediaminenickel(*II*)(2+), 8Cl

(1,2-Ethanediamine-N,N′)nickel(II)(2+), 9Cl

[3580-97-3]

$Ni(NH_2CH_2CH_2NH_2)^{2\ominus}$

M 118.7 (ion)

Studied in aq. soln. in which it is undoubtedly better formulated as Tetraaqua(ethylenediamine)nickel(*II*) (2+), IC-003381.

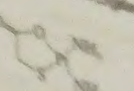
Yokoi, M. *et al., Nippon Kagaku Zasshi, Jpn. J. Chem.*, 1962, **83**, 1192

Ishigure, S. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 3021

$C_2H_8N_2O_2PtS$ IC-003299

Dimethylbis(thiocyanato-*N*)platinum(*II*), 11Cl

[84350-31-2]



M 319.2

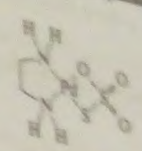
Probably square planar. Synth. from reactions of Dimethylbis(dimethylsulfoxide)platinum(II), IC-019460 + $HSCH_2COOH$. Pale yellow powder. Insol. H_2O, org. solvs.

Kukushkin, Yu.N. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 1787 (*synth, ir*)

$C_2H_8N_2O_2PtS_2$ IC-003300

Ethylenediamine(thiosulfato-*O,S*)platinum(*II*)

[18009-45-1]



M 375.6

Said to be S,O-bonded. Solvated resin is fact to $Pd_2(S_2O_3)_3(en)_2$. Yellow-green solid + $2H_2O$.

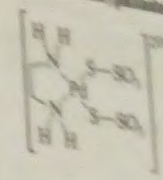
[18009-41-9]

Rychlinkov, D.I. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **48**, 169; *C.A.*, **38**, 4577 (*synth*)

Eskenazi, B. *et al., J. Inorg. Nucl. Chem.*, 1981, **43**, 239 (*synth*)

$C_2H_8N_2O_4PdS_2^{2\ominus}$ IC-003301

Ethylenediaminebis(thiosulfato)palladate(II)(2−)



M 390.7 (ion)

cis-Square planar.

Di-Na salt: [18009-42-0]. Yellow solid.

Di-K salt: Yellow solid + $1H_2O$.

Butylethylenediamine(palladium(2+)) salt:

$C_{12}H_{36}N_4O_4Pd_2S_4$ M 617.3

Air-stable orange plates.

Eskenazi, B. *et al., J. Inorg. Nucl. Chem.*, 1981, **43**, 239 (*synth, cryst struct*)

Beggiato, S. *et al., Acta Crystallogr., Sect. B*, 1975, **31**, 168 (*cryst struct*)

$C_2H_8N_2O_8S_2Zn_3$ IC-003302

Zinc oxide thiocyanate ($Zn_3(OH)_8(SCN)_2$)

Basic zinc thiocyanate

[57034-82-9]

$Zn_3(OH)_8(SCN)_2$

M 579.1

Cryst.

[64763-07-1]

Zurano Hernandez, G. *et al*, *An. Quim.*, 1977, **73**, 820 (*synth, cryst struct*)

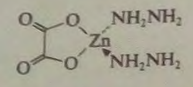
IC-003303

$C_2H_8N_4O_4Zn$

Bis(hydrazine)(oxalato)zinc

[Ethanedioato(2 –)-O,O′]bis(hydrazine-N)zinc, 9CI

[50895-71-1]



M 217.5

Cryst. Insol. EtOH, Et_2O. Dec. at 216°. Forms a monohydrate, which dehydrates at 170°.

[50895-72-2]

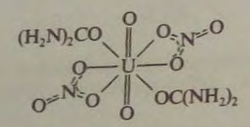
Nikonenko, E.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **18**, 1254 (*synth, thermal anal, powder struct, ir*)
Patil, K.C. *et al*, *Thermochim. Acta*, 1982, **52**, 113 (*synth, ir, thermal anal*)
Nikonenko, E.A. *et al*, *Koord. Khim.*, 1984, **10**, 970 (*ir, raman*)

IC-003304

$C_2H_8N_6O_{10}U$

Bis(nitrato-*O,O′*)dioxobis(urea)uranium(*VI*), 9CI

[18040-79-4]



M 514.1

Hexagonal bipyramidal. Yellow plates.

[17442-31-8]

Gentile, P.S. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 2291.
Bullock, J.I., *J. Inorg. Nucl. Chem.*, 1967, **29**, 2257 (*synth, ir*)
Ellert, G.V. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 1891; 1971, **16**, 3092; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 971; 1971, **16**, 1640 (*synth, ir, luminescence*)
Zarli, B. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 491 (*synth*)
Siracusa, G. *et al*, *Thermochim. Acta*, 1982, **56**, 333 (*thermal dec, ir*)
Alcock, N.W. *et al*, *Acta Crystallogr., Sect. C*, 1990, **46**, 981 (*cryst struct*)

IC-003305

C_2H_9BClN

Chloro(dimethylamine)dihydroboron

Chlorodihydro(N-methylmethanamine)boron, 10CI.
Chloroborane compd. with N-methylmethanamine (1:1), 9CI.
Chloroborane dimethylamine

[52920-74-8]

$Me_2NH—BH_2Cl$

M 93.3

Moisture-sensitive solid. Mp 18°.

Nöth, H. *et al*, *Chem. Ber.*, 1960, **93**, 225 (*synth*)
Beachley, O.T. *et al*, *Inorg. Chem.*, 1975, **14**, 120 (*pmr*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*synth, pmr*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1978, **17**, 1157 (*nmr*)
Balulescu, C.R. *et al*, *Inorg. Chem.*, 1978, **17**, 3707.

IC-003306

C_2H_9BS

(Dimethyl sulfide)trihydroboron

Trihydro[thiobis[methane]]boron, 10CI. Borane compd. with thiobis[methane] (1:1), 9CI. Methyl sulfide compd. with borane, 8CI. Borine compd. with Me_2S. Borane dimethyl sulfide

[13292-87-0]

$Me_2S—BH_3$

M 75.9

Reducing agent which may be used in a variety of solvs. Produced commercially. Moisture-sensitive colourless liq. at r.t. Fp −27°, −38°.

▷ Flammable.

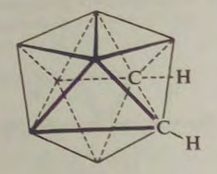
Heal, H.G., *J. Inorg. Nucl. Chem.*, 1960, **12**, 255 (*synth, ir*)
Young, D.E. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 4390 (*nmr*)
Lane, C.F., *Chem. Rev.*, 1976, **76**, 773 (*rev, use*)
Yamamoto, Y. *et al*, *Yuki Gosei Kagaku Kyokaishi*, 1979, **37**, 1008; *CA*, **92**, 139884j (*synth*)
Krishnamurthy, S. *et al*, *J. Org. Chem.*, 1980, **45**, 849.
Brown, H.C. *et al*, *Synthesis*, 1981, 996.
Mancilla, T. *et al*, *Tetrahedron Lett.*, 1982, **23**, 1561.

IC-003307

$C_2H_9B_7$

4,5-Dicarbanonaborane(9), 11CI, 10CI, 9CI, 8CI

[26894-16-6]



M 108.7

closo-. Also called the 1,6-isomer in the lit. Colourless cryst. Mp 108.5-109.5°.

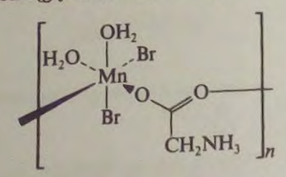
[26998-72-1]

Garrett, P.M. *et al*, *Inorg. Chem.*, 1969, **8**, 1907 (*synth, ir, pmr*)
Dunks, G.B. *et al*, *Inorg. Chem.*, 1970, **9**, 893 (*B-11 nmr*)
Dunks, G.B. *et al*, *Adv. Chem. Res.*, 1973, **6**, 124 (*synth*)
Dunks, G.B. *et al*, *Adv. Chem. Res.*, 1973, **6**, 124 (*synth*)
Lau, K.-K. *et al*, *Inorg. Chem.*, 1976, **15**, 1059 (*microwave, struct, dipole moment*)

IC-003308

$C_2H_9Br_2MnNO_4$

Diaquadibromo(glycine)manganese(*II*)



M 325.8

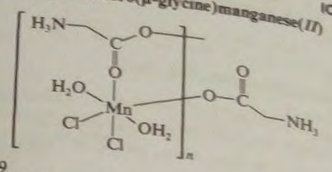
Chain struct. with Mn—O 217-224; Mn—Br 271.1, 263 pm.

Glowiak, T. *et al*, *Bull. Acad. Pol. Sci.*, 1977, **25**, 277; *CA*, **87**, 109850 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 259 (*rev, bibl*)

$C_2H_9Cl_2MnNO_4$

IC-003309

***Catena*-Diaquadichloro(μ-glycine)manganese(*II*)**



M 236.9

Octahedral Mn(*II*) ions are linked by carboxyl bridges of glycine molecules to form spiral chains. Synth. from an aq. soln. of $MnCl_2$ and glycine.

Ciunik, Z. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1212 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 253 (*rev, bibl*)

IC-003310

$C_2H_9N_2OP$

Ethyl phosphorodiamidite, 9CI

Diamidoethoxophosphorus(III)

$EtOP(NH_2)_2$

M 108.0

Yellowish amorph. solid. Mp 140-142° dec.

Becke-Goehring, M. *et al*, *Chem. Ber.*, 1958, **91**, 1188 (*synth, props*)

IC-003311

$C_2H_9N_5NiS_2$

Triamminebis(thiocyanato-*N*)nickel(*II*)

Diisothiocyanatotriamminenickel(II)

$Ni(NCS)_2(NH_3)_3$

M 225.9

Polymeric struct. with Ni bound to 3 NCS and 3 NH_3 (octahedral). Blue-green cryst.

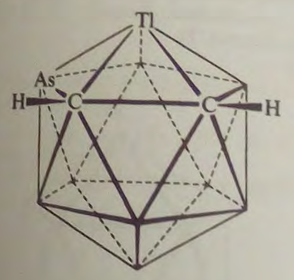
Bohat, G.S., *J. Phys. Chem.*, 1915, **19**, 537 (*synth*)
Porai-Koshits, M.A. *et al*, *Acta Crystallogr.*, 1957, **10**, 784 (*cryst struct*)
Yukhno, E.K., *Zh. Neorg. Khim.*, 1962, **7**, 807; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, **7**, 417 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1968, **C1**, 102 (*rev*)

IC-003312

$C_2H_{10}AsB_8Tl$

[(7,8,9,10,11-η)-Decahydro-7-arsa-8,9-dicarbaundecaborato(1 –)]thallium, 10CI

[72255-14-2]



M 399.8

Proposed struct. shown. Beige solid. Sol. Me_2CO, THF.

Colquhoun, H.M. *et al*, *J. Chem. Res.* (*S*), 1979, 248 (*synth, B-11 nmr*)

IC-003313

$C_2H_{10}BN$

(Dimethylamine)trihydroboron

Trihydro(N-methylmethanamine)boron, 10CI. N-Methylmethanamine compd. with borane (1:1), 9CI. Dimethylamine compd. with borane (1:1), 8CI. Borane dimethylamine

[74-94-2]

$Me_2NH—BH_3$

M 58.9

Used in electroless plating of nickel and copper and in photographic developers. Reducing agent. Solid. Mp 37°. $Bp_{0.01}$ 49°. Dec. at 150°.

▷ IP9450000.

Nöth, H. *et al*, *Chem. Ber.*, 1960, **93**, 928 (*props*)
Brown, M.P. *et al*, *J. Chem. Soc. A*, 1970, 410 (*ir*)
Lloyd, D.R. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 947 (*pe*)
Nöth, H. *et al*, *Chem. Ber.*, 1974, **107**, 3070 (*nmr*)
Beachley, O.T. *et al*, *Inorg. Chem.*, 1975, **14**, 120 (*pmr*)
Kovar, R.A. *et al*, *Inorg. Chem.*, 1975, **14**, 2239 (*crystal, ir*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*pmr*)

IC-003314

$C_2H_{10}BP$

(Dimethylphosphine)trihydroboron, 10CI

Dimethylphosphine, compd. with borane (1:1), 9CI, 8CI. Borane dimethylphosphine. Dimethylphosphine borine

[4268-35-3]

$Me_2PH—BH_3$

M 75.8

Liq. Mp −22.6°. Slowly dehydrogenates on heating at 150°.

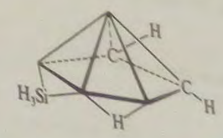
Burg, A.B. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 3872 (*synth*)
Phillips, W.D. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 4496 (*nmr*)
Verkade, J.G. *et al*, *Inorg. Chem.*, 1964, **3**, 884 (*pmr*)
Cowley, A.H. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 6815 (*nmr*)
Drake, J.E. *et al*, *J. Chem. Soc. A*, 1971, 2074 (*pmr, ir, raman*)
Rapp, B. *et al*, *Inorg. Chem.*, 1973, **12**, 2868 (*nmr*)

IC-003315

$C_2H_{10}B_4Si$

μ-Silyl-2,3-dicarbahexaborane(8), 9CI

[38999-41-6]



M 105.4

Colourless liq.

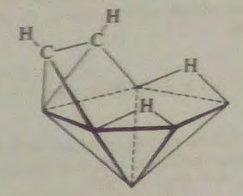
Thompson, M.L. *et al*, *Inorg. Chem.*, 1972, **11**, 1925 (*ir, nmr, ms, struct, synth*)

IC-003316

$C_2H_{10}B_8$

Dicarbaoctaborane(10), 11CI, 9CI

[50442-30-3]



M 98.9

nido-. One possible isomeric form shown. Air sensitive colourless liq. Dec. at r.t. in liq. phase to $C_2B_6H_8$ and $C_2B_5H_7$.

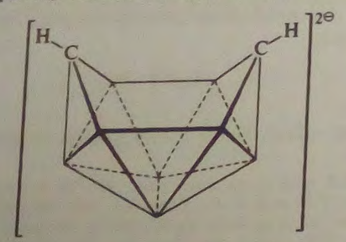
[99532-11-3]

Gotcher, A.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 7514 (*synth, ir, pmr, B-11 nmr, ms*)
Reilly, T.J. *et al*, *Inorg. Chem.*, 1974, **13**, 1250 (*synth*)
Corcoran, E.W. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 7446 (*synth*)

IC-003317

$C_2H_{10}B_8^{2\ominus}$

Decahydro-6,9-dicarbadecaborate(2−), 9CI



M 120.5 (ion)

nido-. Originally thought to be 5,7-isomer.

Di-Na salt: [39430-65-4].

$C_2H_{10}B_8Na_2$ M 166.5

Colourless solid. Sol. THF, H_2O, Me_2CO.

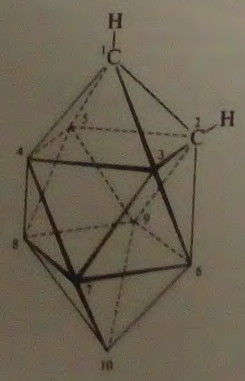
Stibr, B. *et al*, *Collect. Czech. Chem. Commun.*, 1973, **38**, 338; 1984, **49**, 1891 (*synth, ir, B-11 nmr*)

IC-003318

$C_2H_{10}B_8$

1,2-Dicarbadecaborane(10), 10CI

[41655-27-0]



M 120.5

Cryst. Mp 182° (174°).

Rietz, R.R. *et al*, *J. Organomet. Chem.*, 1973, **63**, 1 (*nmr, synth*)
Plešek, J. *et al*, *Collect. Czech. Chem. Commun.*, 1974, **39**, 821 (*ms, synth*)

IC-003319

$C_2H_{10}B_8$

1,6-Dicarbadecaborane(10), 10CI

[23704-81-6]

M 120.5

closo-. Cryst. Mp 146°. Dipole moment 2.22D.

Garrett, P.M. *et al*, *Inorg. Chem.*, 1969, **8**, 1907 (*synth, ir, nmr*)

IC-003320

$C_2H_{10}B_8$

1,10-Dicarbadecaborane(10), 10CI

[23653-23-8]

M 120.5

closo-. Cryst. Mp 162°.

Garrett, P.M. *et al*, *Inorg. Chem.*, 1969, **8**, 1907 (*synth, ir, nmr*)
Leites, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1975, 1866 (*ir, raman*)
Atavin, E.G. *et al*, *J. Mol. Struct.*, 1980, **65**, 259 (*ed*)

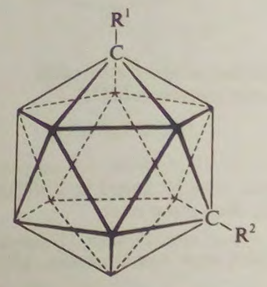
IC-003321

$C_2H_{10}B_{10}Br_2Hg_2$

Dibromo-μ-1,7-dicarbadodecaboran(12)-1,7-diyldimercury, 8CI

1,7-Bis(bromomercuri)-m-*carborane*. *1,7-Bis(bromomercuri) neobarene*

[23704-89-4]



$R^1 = R^2 = HgBr$

M 703.1

Cryst. (toluene). Mp 314-316°.

Zakharkin, L.I. *et al*, *J. Organomet. Chem.*, 1967, **7**, 385 (*synth*)

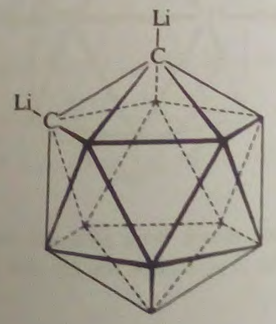
IC-003322

$C_2H_{10}B_{10}Li_2$

μ-1,2-Dicarbadodecaborane(12)-1,2-diyldilithium, 10CI

Dilithium-1,2-dicarbadodecaborate(2−). *1,2-Dilithio-1,2-dicarbadodecaborane(12)*

[22220-85-5]



M 156.0

closo-. Precursor to many σ-substituted derivs. of 1,2-$C_2B_{10}H_{12}$.

Heying, T. *et al*, *Inorg. Chem.*, 1963, **2**, 1097 (*synth*)
Grafstein, D. *et al*, *Inorg. Chem.*, 1963, **2**, 1120 (*synth*)

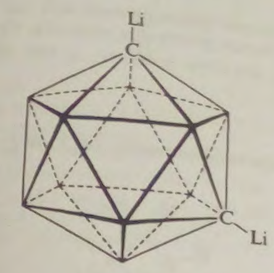
IC-003323

$C_2H_{10}B_{10}Li_2$

μ-1,7-Dicarbadodecaborane(12)-1,7-diyldilithium, 10CI

Dilithium-1,7-dicarbadodecaborate(2−). *1,7-Dilithio-1,7-dicarbadodecaborane(12)*

[17217-89-9]



M 156.0

closo-. Precursor to many σ-substituted derivs. of 1,7-$C_2B_{10}H_{12}$. Sol. Et_2O, C_6H_6, THF.

Grafstein, D. *et al*, *Inorg. Chem.*, 1963, **2**, 1128.
Stanko, V. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1971, **41**, 2053.

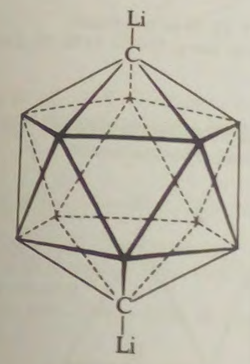
IC-003324

$C_2H_{10}B_{10}Li_2$

μ-1,12-Dicarbadodecaborane(12)-1,12-diyldilithium, 10CI

Dilithium-1,12-dicarbadodecaborate(2−). *1,12-Dilithio-1,12-dicarbadodecaborane(12)*

[23087-97-0]



M 156.0

closo-. Precursor to many σ-substituted derivs. of 1,12-$C_2B_{10}H_{12}$. Sol. liq. NH_3.

Zakharkin, L. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1968, 2532 (*synth*)
Stanko, V. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1971, **41**, 2053 (*synth*)

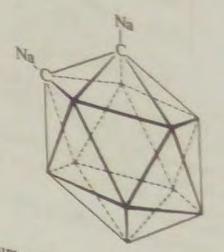
IC-003325

$C_2H_{10}B_{10}Na_2$

μ-1,2-Dicarbadodecaborane(12)-1,2-diyldisodium, 10CI

Disodium-1,2-dicarbadodecaborate(2−). *1,2-Disodio-1,2-dicarbadodecaborane(12)*

[56310-81-7]



M 188.1

closo-. Precursor to many σ-substituted $1,2\text{-}C_2B_{10}H_{12}$ derivs. Sol. Et_2O.

Zakharkin, L. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1964, 546 (*synth*)
Zakharkin, L., *Tetrahedron Lett.*, 1964, 2255 (*synth*)

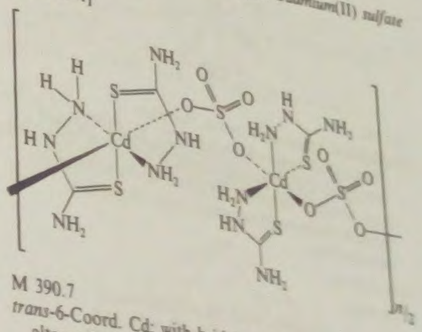
IC-003326

$C_2H_{10}CdN_6O_4S_3$

Bis(hydrazinecarbothioamide-N^2,S)[sulfato(2−)-O]cadmium

Bis(thiosemicarbazide)cadmium sulfate. *Cadmium(II) sulfate bis(thiosemicarbazide)*

[57193-96-1]



M 390.7

trans-6-Coord. Cd; with bridging SO_4 groups and alternating *cis* and *trans* arrangements of the two thiosemicarbazide units. Cryst. (H_2O).

[57193-95-0]

Larsen, E. *et al*, *Acta Chem. Scand., Ser. A*, 1975, **29**, 481 (*synth, cryst struct*)
Bauer, R. *et al*, *J. Chem. Phys.*, 1979, **70**, 4117.
Mirzubaimov, B. *et al*, *Koord. Khim.*, 1985, **11**, 596 (*ir*)

IC-003327

$C_2H_{10}Cl_2FeN_2$

Dichlorobis(methylamine)iron(II)

Iron(II) chloride bis(methylamine). *Ferrous chloride bis(methylamine)*

M 188.8

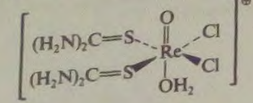
Struct. unknown. Unlikely to be simple 1:1 complex. Synth. from $FeCl_2$ or $FeCl_3$ + $MeNH_2$. White solid. V moisture and air-sensitive. Insol. or reacts with most solvs. $\mu_{eff} = 4.9\mu_B$. Dec. at 120°.

McGregor, W.R. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1027 (*synth, ir, magnetism*)

IC-003328

$C_2H_{10}Cl_2N_4O_2ReS_2^{\oplus}$

Aquadichlorooxobis(thiourea)rhenium(*V*)(1+), 9CI



trans,cis,cis-form

M 443.3 (ion)
Octahedral. Mean interatomic distances: Re=O 145.4, Re—S 234.8, Re—ON 223.1, Re—Cl 236.5 pm.

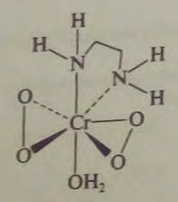
trans,cis,cis-form [60869-18-3]
Oxoaqua-cis-dichloro-cis-bis(thiourea)rhenium(V)(*1+*)
Chloride: Synth. from $KReO_4$ and thiourea in conc. HCl. Blue needles (conc. HCl).

Lis, T., *Acta Crystallogr., Sect. B*, 1976, **32**, 2707 (*cryst struct*)

IC-003329

$C_2H_{10}CrN_2O_5$

Aqua(1,2-ethanediamine-*N,N'*)diperoxychromium(*IV*), 11CI, 10CI
Aqua(ethylenediamine)diperoxochromium(IV).
Diperoxoaquo(ethylenediamine)chromium(IV)
[17192-14-2]



M 194.1
Pentagonal bipyramidal struct. See also Triamminediperoxychromium(*IV*), IC-017715 and Tris(cyano-*C*)diperoxychromate(*IV*)(3−), IC-003551 for relat. compds. Intermed. in synth. of chromium(*III*) amine complexes. Olive green cryst., forms a monohydrate.

▷ May explode.

[17168-84-2]

Stomberg, R., *Ark. Kemi.*, 1965, **24**, 47 (*cryst struct*)
Ghosh, S.K. *et al*, *Inorg. Chem.*, 1988, **27**, 4224, 4228.
Ranganathan, C.K. *et al*, *Inorg. Chem.*, 1989, **28**, 1306.

IC-003330

$C_2H_{10}N_3OP$

N,N-Dimethylphosphoric triamide, 9CI
N,N-Dimethyltriamidooxophosphorus(V)
[19316-37-1]

$Me_2NP(O)(NH_2)_2$

M 123.0
Efficient plant fertiliser. Cryst. (Me_2CO). Mp 119°. Low stability at pH 4-8. Urease inhibitor.

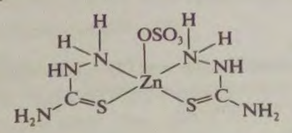
N',N''-Di-Me: [16853-36-4]. N,N,N',N''-*Tetramethylphosphoric triamide*
$C_4H_{14}N_3OP$ M 151.1
Oil which solidifies. Mp 38°. Bp_2 145°.

Goehring, M. *et al*, *Chem. Ber.*, 1956, **89**, 1768 (*synth*)
Terry, P.H. *et al*, *J. Agric. Food Chem.*, 1973, **21**, 500 (*deriv*)
Baldwin, M.A. *et al*, *Org. Mass Spectrom.*, 1977, **12**, 279 (*synth, deriv, ms*)
Roemer, W. *et al*, *CA*, 1979, **91**, 73618 (*props*)

IC-003331

$C_2H_{10}N_6O_4S_3Zn$

(Sulfato)bis(thiosemicarbazide)zinc
Bis[hydrazinecarbothioamide-N^2,S*][sulfato(2−)-O]zinc, 11CI*
[70804-56-7]



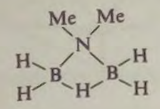
M 343.7
Struct. is a distorted square-pyramid with the thiosemicarbazide groups in a *cis*-config. Cryst. (H_2O).

Larsen, S. *et al*, *Acta Chem. Scand., Ser. A*, 1985, **39**, 441 (*cryst struct*)

IC-003332

$C_2H_{11}B_2N$

[μ-(Dimethylamino)]diborane(6), 10CI, 9CI, 8CI
[23273-02-1]



M 70.7
Synthetic intermed. Volatile liq., sensitive to air and moisture; can be stored at 25° for months in sealed tube *in vacuo*. Sol. ethers, aromatic hydrocarbons, dec. in protic solvs. V.p. 101 mm (0°).

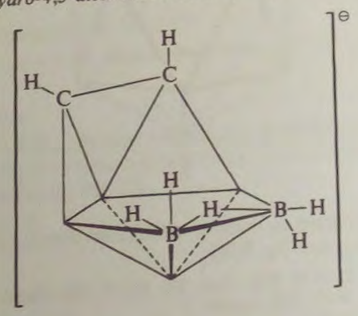
▷ Toxic, spontaneously flammable. IP9700000.

Keller, P.C., *J. Am. Chem. Soc.*, 1969, **91**, 1231 (*synth*)
Spielman, J.R., *J. Chem. Educ.*, 1970, **47**, 225 (*synth*)
Cohen, E.A. *et al*, *Inorg. Chem.*, 1973, **12**, 1570 (*microwave*)
Allison, D.A. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1973, **1**, 269 (*pe*)
Leleu, J., *Cah. Notes Doc.*, 1977, **86**, 97; *CA*, **88**, 109657n (*haz, rev*)
Inorg. Synth., 1977, **17**, 34 (*synth, props*)
Balulescu, C.R. *et al*, *Inorg. Chem.*, 1978, **17**, 3707 (*nmr*)

IC-003333

$C_2H_{11}B_6^{\ominus}$

Undecahydro-3,8-dicarbaoctaborate(1−), 12CI
Undecahydro-4,5-dicarbaoctaborate(1−)



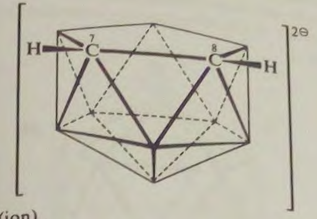
M 99.9 (ion)
arachno-.
Me_4N salt: [125937-25-9].
Colourless cryst. (toluene/MeCN). Sol. MeCN.

Jelinek, T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 804 (*synth, pmr, B-11 nmr*)

$C_2H_{11}B_9^{2\ominus}$

IC-003334

Undecahydro-7,8-dicarbaundecaborate(2−), 11CI, 10CI, 9CI
[56902-43-3]



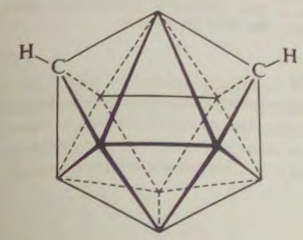
M 132.4 (ion)
nido-. Many complexes of this anion are known.
Di-Na salt: [12541-50-3].
$C_2H_{11}B_9Na_2$ M 178.3
Prepd. *in situ* as colourless soln. in THF.

Warren, L.F. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 470 (*synth*)
Hawthorne, M.F., *Acc. Chem. Res.*, 1968, **1**, 281 (*rev, bibl*)
Hawthorne, M.F. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 879, 896 (*synth*)

IC-003335

$C_2H_{11}B_9$

2,3-Dicarbaundecaborane(11), 11CI, 10CI, 9CI, 8CI
[33362-09-3]



M 132.4
closo-. Known as 1,8- or 9,10- isomers in early lit.
Colourless cryst. (pentane). Sol. $CHCl_3$, CS_2, pentane. Mp 212-213°.

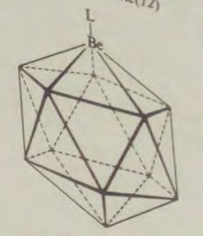
[17764-84-0]

Tebbe, F.N. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 869 (*synth, ir, pmr, B-11 nmr*)
Todd, L.J. *et al*, *Pure Appl. Chem.*, 1972, **30**, 587 (*cmr*)
Echeistova, A.I. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1974, **15**, 141 (*dipole moment*)
Scholer, F.R. *et al*, *Inorg. Chem.*, 1979, **18**, 921 (*B-11 nmr*)

IC-003334

$C_2H_{11}B_9Be$

[Undecahydro-7,8-dicarbaundecaborato(2−)]beryllium
1,2-Dicarba-3-berylladodecaborane(12)



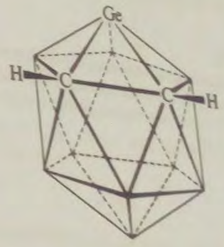
M 141.4 L = NMe_3 or OEt_2
Obt. as closo-complex.
Me_3N complex: [31743-01-8]. 3-(*Trimethylammonium*)*undecahydro-1,2-dicarba-3-berylladodecaborate.* (*Trimethylamine*)[*undecahydro-7,8-dicarbaundecaborato*(2−)]*beryllium*
$C_5H_{20}B_9BeN$ M 200.5
Colourless cryst. (CH_2Cl_2/pentane). Sol. CH_2Cl_2. Mp 221-223° dec.
Et_2O complex:
$C_6H_{21}B_9BeO$ M 215.5
Extremely air- and water-sensitive cryst. (CH_2Cl_2/pentane). Sol. CH_2Cl_2. Mp 120-121°.

Popp, G. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 6553 (*synth, pmr, B-11 nmr, ms*)
Popp, G. *et al*, *CA*, 1971, **74**, 141937a.
Popp, G. *et al*, *Inorg. Chem.*, 1971, **10**, 391 (*synth, pmr*)

IC-003337

$C_2H_{11}B_9Ge$

1,2-Dicarba-3-germadodecaborane, 8CI
1-Germa-2,3-dicarba-closo-dodecacarborane
[27071-52-9]



M 205.0
White solid (C_6H_6). Sol. C_6H_6. Subl. 80° *in vacuo*. Dec. at 352°.

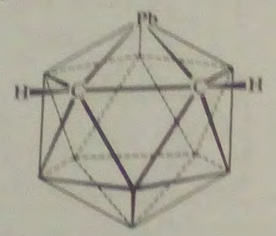
Rudolph, R.W. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 3351.

$C_2H_{11}B_9Pb$ IC-003338

1,2-Dicarba-3-plumbadodecacarborane(11), 8Cl

1-Plumba-2,3-dicarba-closo-dodecacarborane

[27071-51-8]



M 339.6

closo-. Yellow solid (C_2H_6). Subl. 250° *in vacuo*. Dec. at 250°.

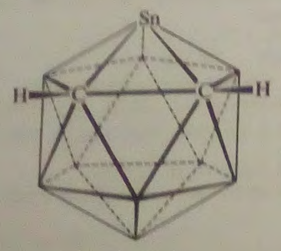
Rudolph, R.W. *et al, J. Am. Chem. Soc.*, 1970, **92**, 3351.

$C_2H_{11}B_9Sn$ IC-003339

1,2-Dicarba-3-stannadodecaborane

1-Stanna-2,3-dicarbadodecacarborane

[23151-46-4]



M 251.1

White solid (C_6H_6). Sol. C_6H_6. Subl. 140° *in vacuo*. Dec. at 210°.

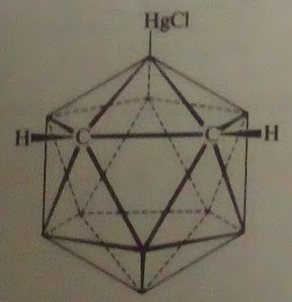
Rudolph, R.W. *et al, J. Am. Chem. Soc.*, 1970, **92**, 3351.

$C_2H_{11}B_{10}ClHg$ IC-003340

Chloro-1,2-dicarbadodecaboran(12)-3-ylmercury

Chloro[undecahydro-1,2-dicarbadodecaborato(1−)-B^3]mercury, 9Cl. 3-Chloromercuri-o-carborane. o-Carboran-3-ylmercury chloride

[38268-75-6]



M 379.2

closo-. Cryst. (C_6H_6). Mp 296-297°.

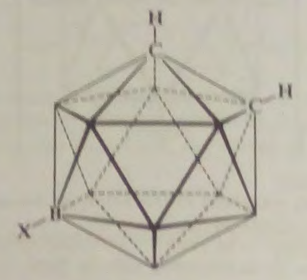
Zakharkin, L.I. *et al, J. Organomet. Chem.*, 1972, **40**, 15 (*synth*)

$C_2H_{11}B_{10}ClHg$ IC-003341

Chloro(1,2-dicarbadodecaboran(12)-9-yl)mercury, 10Cl, 9Cl

1,2-Dicarbadodecaboran(12)-9-ylmercury chloride. o-Carboran-9-ylmercury chloride. o-Carboran-9-yl-chloromercury. 9-Chloromercuri-o-carborane

[59993-36-1]



X = HgCl

M 379.2

Cryst. (toluene). Mp 263-264°.

Bregadze, V.I. *et al, J. Organomet. Chem.*, 1976, **112**, 249; 1977, **136**, 281 (*synth*)

Kampel', V.Ts., *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1978, **27**, 1318 (*polarography*)

Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)

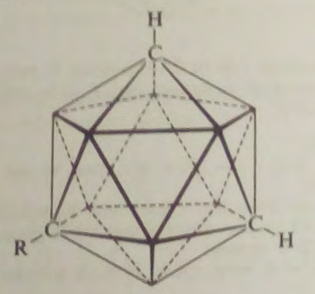
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1981, **30**, 1670 (*ir, raman*)

$C_2H_{11}B_{10}ClHg$ IC-003342

Chloro-1,7-dicarbadodecaboran(12)-9-ylmercury, 10Cl

1,7-Dicarbadodecaboran(12)-9-ylmercury chloride. m-Carboran-9-ylmercury chloride. m-Carboran-9-ylchloromercury. 9-Chloromercuri-m-carborane

[59993-37-2]



R = HgCl

M 379.2

Cryst. (toluene or *m*-xylene). Mp 266-267°.

Bregadze, V.I. *et al, J. Organomet. Chem.*, 1976, **112**, 249; 1977, **136**, 281 (*synth*)

Kampel', V.Ts., *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1978, **27**, 1318 (*electrochem*)

Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)

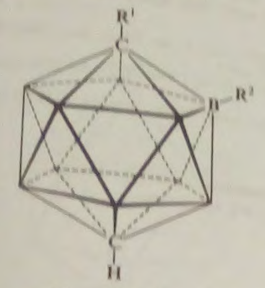
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1981, **30**, 1670 (*ir, raman*)

$C_2H_{11}B_{10}ClHg$ IC-003343

Chloro-1,12-dicarbadodecaboran(12)-2-ylmercury, 10Cl

1,12-Dicarbadodecaboran(12)-2-ylmercury chloride. p-Carboranyl-2-chloromercury. p-Carboran-2-ylmercury chloride. 2-Chloromercuri-p-carborane

[64616-55-3]



R^1 = H, R^2 = HgCl

M 379.2

Cryst. (toluene). Mp 259-260°.

Bregadze, V.I. *et al, J. Organomet. Chem.*, 1977, **136**, 281 (*synth*)

Kampel', V.Ts., *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1978, **27**, 1318 (*polarog*)

Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)

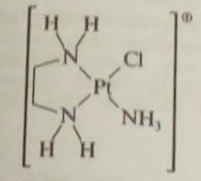
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1981, **30**, 1670 (*ir, raman*)

$C_2H_{11}ClN_2Pt^{\oplus}$ IC-003344

Amminechloro(ethylenediamine)platinum(*II*)(1+)

Amminechloro(1,2-ethanediamine-N,N′)platinum(II)(*1+*), *9Cl*

[61130-25-4]



M 307.6 (ion)

Probably square planar. Synth. from $[Pt(en)(NH_3)_2]^{2\oplus}$ + HCl.

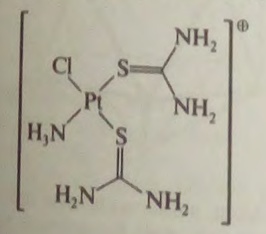
Chloride: [73309-16-7].

Fluffy white cryst.

Bonivento, M. *et al, Inorg. Chem.*, 1980, **19**, 1743 (*synth, reactions*)

$C_2H_{11}ClN_5PtS_2^{\oplus}$ IC-003345

Ammine(chloro)bis(thiourea)platinum(*II*)(1+)



M 399.8 (ion)

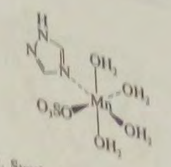
Intermediate in reaction of *cis*-form of Diamminedichloroplatinum(*II*), IC-016643 + thiourea to give Tetrakis(thiourea)platinum(*II*)(2+), IC-004393. Presumed *cis*- square planar struct. but no recent studies. Intermed in Kurnakov test for distinguishing between *cis* and *trans*- $Pt(NH_3)_2X_2$.

Compr. Coord. Chem., Pergamon, Oxford, 1987, **2**, 639 (*mech*)

$C_2H_{11}MnN_5O_9S$ IC-003346

Tetraaqua[sulfato(2−)-*O*][(1*H*-1,2,4-triazole-N^4)manganese(*II*), 10Cl

[78407-64-4]



M 292.1

cis-Octahedral. Synth. from conc. aq. solns. of $MnSO_4$ and 1,2,4-triazole at r.t. Air-stable.

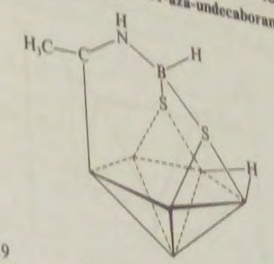
Haasnoot, J.G. *et al, Z. Naturforsch., B*, 1977, **32**, 1421 (*synth, ir*)

Gorter, S. *et al, Acta Crystallogr., Sect. B*, 1981, **37**, 1214 (*synth, cryst struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 65 (*rev, bibl*)

$C_2H_{12}B_7NS_2$ IC-003347

5-Methyl-5-carba-7,14-dithia-11-aza-undecaborane(7)



M 189.9

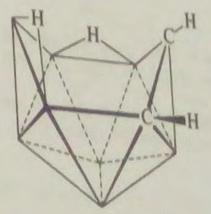
hypho-. Colourless cryst. by subl. Sol. hexane, C_6H_6. Mp 128-129°. Subl. 60° *in vacuo*.

Kang, S.O. *et al, Inorg. Chem.*, 1989, **28**, 2339 (*synth, ir, pmr, B-11 nmr, ms, cryst struct*)

$C_2H_{12}B_8$ IC-003348

5,6-Dicarbadecaborane(12), 11Cl, 10Cl, 9Cl

[34640-08-9]



M 122.6

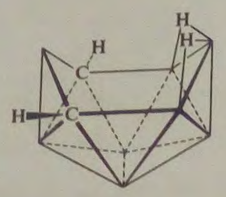
nido-. Mod. air stable colourless solid. Sol. hexane, THF. Mp 98-99°.

[41655-26-9]

Plesek, J. *et al*, *Chem. Ind. (London)*, 1971, 1267 (*synth, ir, pmr, B-11 nmr, uv, ms*)
Stibr, B. *et al*, *Collect. Czech. Chem. Commun.*, 1973, **38**, 338 (*synth*)
Rietz, R.R. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6254 (*synth, ir, B-11 nmr, ms*)
Plesek, J. *et al*, *Collect. Czech. Chem. Commun.*, 1974, **39**, 821 (*synth, B-11 nmr, ms*)
Lawrence, S.H. *et al*, *Inorg. Chem.*, 1986, **25**, 367 (*synth*)

IC-003349

$C_2H_{12}B_8$
5,7-Dicarbadecaborane(12), 10CI, 8CI
[31387-16-3]

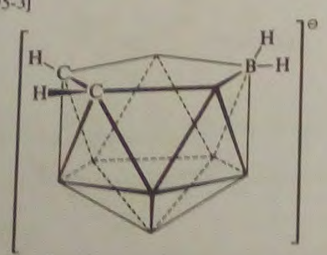


M 122.6
nido-. Air and moisture sensitive colourless solid. Sol. CS_2. Mp 139-140°.

Garrett, P.M. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 1265 (*synth, ir, pmr, B-11 nmr*)

IC-003350

$C_2H_{12}B_9^{\ominus}$
Dodecahydro-7,8-dicarbaundecaborate(1 –), 11CI, 10CI, 9CI, 8CI
[11130-95-3]



M 133.4 (ion)
nido-. Known as the (3)-1,2-isomer in early lit.
K salt: [12304-72-2].
$C_2H_{12}B_9K$ M 172.5
Often used as a source of $C_2B_9H_{12}^{\ominus}$ for metal complex formation. Colourless solid. Sol. H_2O, alcohols; insol. Et_2O. Quite hygroscopic.
Me_4N salt: [12304-89-1].
Colourless solid. Sol. alcohols, ketones, nitriles; insol. H_2O.

[12385-59-0]

Garrett, P.M. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 5016 (*synth*)
Hawthorne, M.F. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 862 (*synth, ir, pmr, B-11 nmr*)
Inorg. Synth., 1983, **22**, 231 (*synth, pmr, B-11 nmr, rev, bibl*)
Buchanan, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1990, 677 (*cryst struct*)

IC-003351

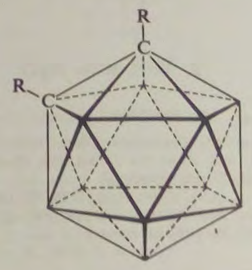
$C_2H_{12}B_9^{\ominus}$
Dodecahydro-7,9-dicarbaundecaborate(1 –), 11CI, 10CI, 9CI, 8CI
[11093-02-0]

M 133.4 (ion)
nido-. Known as the (3)-1,7-isomer in early lit.
Cs salt: [12305-33-8].
$C_2H_{12}B_9Cs$ M 266.3
Colourless solid. Sol. Me_2CO, EtOH.
Me_3NH salt: [54531-56-5].
Colourless solid. Sol. MeCN, Me_2CO, alcohols; insol. H_2O.

Hawthorne, M.F. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 862 (*synth, ir, pmr, B-11 nmr*)
Howe, D.V. *et al*, *Inorg. Chem.*, 1971, **10**, 2516 (*synth, ir, B-11 nmr*)
Todd, L.J. *et al*, *Inorg. Chem.*, 1975, **14**, 1249 (*B-11 nmr*)

IC-003352

$C_2H_{12}B_{10}$
1,2-Dicarbadodecaborane(12), 10CI
o-Carborane. *o-Carbaborane*
[16872-09-6]



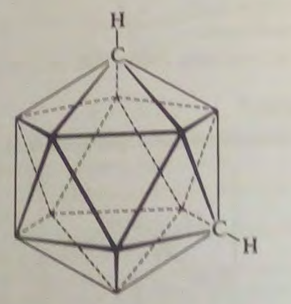
R = H

M 144.2
closo-. Shows high temp. stability; forms many C- and B-substituted derivs. White solid (pentane). Sol. aromatic solvs. Mp 320° (evacuated sealed tube).

Schroeder, H. *et al*, *Inorg. Chem.*, 1963, **2**, 1092 (*ir*)
Potenza, J. *et al*, *Inorg. Chem.*, 1964, **3**, 1673 (*cryst struct*)
Schroeder, H. *et al*, *Inorg. Chem.*, 1966, **5**, 693 (*nmr*)
Inorg. Synth., 1967, **10**, 93; 1968, **11**, 19 (*synth*)
Tupciauskas, V. *et al*, *Zh. Strukt. Khim.*, 1972, **13**, 823 (*pmr*)

IC-003353

$C_2H_{12}B_{10}$
1,7-Dicarbadodecaborane(12), 10CI
m-Carborane. *m-Carbaborane*. *Neocarborane*
[16986-24-6]

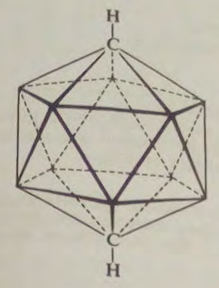


M 144.2
closo-. Highly temp. stable carborane unit which forms many stable derivs., used for polymer formation. White cryst. Mp 273°.
▷ HS9290000.

Grafstein, D. *et al*, *Inorg. Chem.*, 1963, **2**, 1128 (*synth, ms*)

Schroeder, H. *et al*, *Inorg. Chem.*, 1966, **5**, 693 (*nmr*)
Beall, H. *et al*, *Inorg. Chem.*, 1967, **6**, 874 (*cryst struct*)
Ditter, J. *et al*, *Inorg. Chem.*, 1970, **9**, 889 (*synth*)
Tupciauskas, V. *et al*, *Zh. Strukt. Khim.*, 1972, **13**, 823 (*pmr*)

$C_2H_{12}B_{10}$
1,12-Dicarbadodecaborane(12), 10CI IC-003354
p-Carborane. *p-Carbaborane*
[20644-12-6]



M 144.2
closo-. Highly temp. stable carborane unit which forms many stable derivs., used for polymer formation. White solid. Mp 260°. Subl.$_{0.1}$ 110°.

Papetti, S. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 2295 (*synth, nmr*)
Schröder, H. *et al*, *Inorg. Chem.*, 1966, **5**, 693 (*nmr*)
Tupciauskas, V. *et al*, *Zh. Strukt. Khim.*, 1972, **13**, 823 (*pmr*)

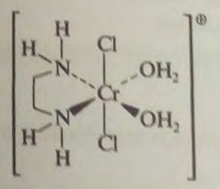
$C_2H_{12}Cl_2CoN_4$ IC-003355
Dichlorobis(methylhydrazine-*N'*)cobalt(*II*)

$[(MeNHNH_2)_2CoCl_2]_n$

M 221.9
Probably octahedral polymeric struct. Prepared from anhydrous $CoCl_2$ and excess anhydrous hydrazine. Pale violet solid. Paramagnetic.

Nicholls, D. *et al*, *J. Chem. Soc. A*, 1966, 950 (*synth, ir, uv, magnetism*)

$C_2H_{12}Cl_2CrN_2O_2^{\oplus}$ IC-003356
Diaquadichloro(ethylenediamine)chromium(*III*)(1+), 8CI
*Diaquadichloro(1,2-ethanediamine-*N,N'*)chromium(1+), 11CI, 9CI*
[16702-63-9]



M 219.0 (ion)
Octahedral struct. with *trans* chlorines.
Chloride: [24458-69-3]. *Weinmann's blue*
$C_2H_{12}Cl_3CrN_2O_2$ M 254.4
Blue cryst. Sol. H_2O, dil. acids, MeOH, EtOH; insol. 2-propanol.

[55401-10-0]

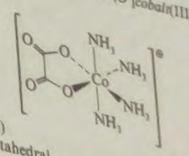
House, D.A. *et al*, *Inorg. Chem.*, 1966, **5**, 840 (*synth, uv-vis*)
Stomberg, R. *et al*, *Acta Chem. Scand.*, 1969, **23**, 343 (*cryst struct*)

$C_2H_{13}Cl_2N_4Ni$ IC-003357
Dichlorobis(methylhydrazine)nickel, 8CI
[29469-14-5]

M 221.7 $NiCl_2(MeNHNH_2)_2$
Believed to have 6-coord. nickel, prob. with hydrazine bridges. Formed by direct synth. or on heating 6:1 complex at 100°. Blue cryst. (EtOH). μ_{eff} = 2.80μ_B.

Nicholls, D. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 2211 (*synth, uv-vis, magnetism*)

$C_2H_{12}CoN_4O_4^{\oplus}$
Tetraammineoxalatocobalt(*III*)(1+) IC-003358
Tetraammine[ethanedioato(2–)-O,O']cobalt(III)(1+), 10CI
[21560-02-1]



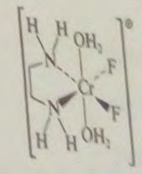
M 215.0 (ion)
Presumed octahedral.
Chloride: Sol. H_2O.

Bark, L.S. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1661 (*synth, kinetics*)

$C_2H_{12}CoN_6S_2^{\oplus}$
Tetraamminebis(thiocyanato-*N*)cobalt(*III*)(1+), 10CI IC-003359
Tetraamminediisothiocyanatocobalt(III)(1+)
$[Co(NCS)_2(NH_3)_4]^{\oplus}$
M 243.2 (ion)
Chloride: [81891-96-5].
$C_2H_{12}ClCoN_6S_2$ M 278.6
Brick red solid.
Acetate: [75657-59-9].
Obt. as 1:1 complex with HOAc.

Westcott, T.J. *et al*, *Aust. J. Chem.*, 1980, **33**, 1853 (*cryst struct*)
Chamberlain, M.M. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 6412 (*ir*)
Kanamori, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 764 (*synth, ir, raman*)

$C_2H_{12}CrF_2N_2O_2^{\oplus}$
Diaqua(ethylenediamine)difluorochromium(*III*)(1+), 8CI IC-003360
*Diaqua(1,2-ethanediamine-*N,N'*)difluorochromium(1+), 11CI, 10CI, 9CI. Diaquadifluoro(ethylenediamine) chromium(III)*
[34398-38-4]



M 186.1 (ion)
Starting complex for synth. of $[CrF_2(O\text{-}O)(en)]^{\oplus}$ complexes.
Chloride: [86275-70-9].
Synth. by ion-exchange from bromide. Violet cryst.
Bromide: [80303-14-6].

Synth. from *cis*-$[Cr(en)_2F_2][Cr(en)F_4].H_2O$ and HBr at r.t. Purple cryst. (H_2O).

[70166-18-6, 70222-96-7]

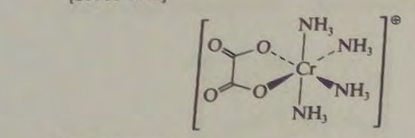
Vaughn, J.W., *Synth. React. Inorg. Metal-Org. Chem.*, 1979, **9**, 1 (*synth*)
Kaizaki, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 3191 (*ir, uv-vis, synth*)
Vaughn, J.W., *J. Crystallogr. Spectrosc. Res.*, 1983, **13**, 231 (*cryst struct*)

$C_2H_{12}CrN_4O_4^{\oplus}$ IC-003361

Tetraammineoxalatochromium(*III*)(1+), 8Cl

Tetraammine[ethanedioato(2−)-O,O′]chromium(1+), 11Cl, 10Cl, 9Cl

[28101-87-3]



M 208.1 (ion)

Chloride: [15275-11-3].
Red orange cryst. (10% aq. NaCl).

Bromide: [14264-11-0].
Red-orange cryst. (10% aq. NaBr).

Nitrate: [14096-59-4].
Synth. from $[Cr(OH_2)(NH_3)_5](NO_3)_3$ and aq. $H_2C_2O_4$ and $K_2C_2O_4$ at 70°. Red orange cryst. (5-10% aq. KNO_3). Forms a monohydrate.

Perchlorate: [42281-04-9].
Synth. from oxalic acid and $[Cr(OH_2)(NH_3)_5](ClO_4)_3$.

Dithionate (2:1): [54538-45-3].
Red solid.

Diamminebis(oxalato)chromate(1−): see *Diamminebis(oxalato)chromate*(III)(1−), *IC-004007*
[19441-07-7]

Kyuno, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 1848 (*synth, uv*)
Hoppenjans, D.W. *et al*, *Inorg. Chem.*, 1969, **8**, 505.
Davies, R. *et al*, *Inorg. Chem.*, 1971, **10**, 2432 ($Cr^{2\oplus}$ *reduction*)
Davies, M.B. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 3354 (*aquation*)
Casabo, J. *et al*, *Inorg. Chim. Acta*, 1974, **11**, 149 (*synth, ir*)
Andriessen, W.T.M., *Inorg. Chem.*, 1976, **15**, 2044 (*esr*)

$C_2H_{12}CrN_4^{\oplus}$ IC-003362

Tetraamminebis(cyano-*C*)chromium(*III*)(1+), 11Cl, 10Cl

Tetraamminedicyanochromium(III)(1+)

[76299-50-8]

$[Cr(CN)_2(NH_3)_4]^{\oplus}$

M 172.1 (ion)

cis-form

Perchlorate: [77981-99-8].
Yellow cryst.
▷ Potentially explosive.

trans-form

Perchlorate: [77904-36-0].
Lemon yellow cryst. (H_2O).

[77981-98-7]

Riccieri, P. *et al*, *Inorg. Chem.*, 1981, **20**, 1432, 3722; 1985, **24**, 441 (*synth, uv, aquation*)
Zinato, E. *et al*, *Inorg. Chem.*, 1984, **23**, 1138 (*photochem*)

$C_2H_{12}CrN_6S_2^{\oplus}$ IC-003363

Tetraamminebis(thiocyanato-*N*)chromium(*III*)(1+), 11Cl, 10Cl, 9Cl

Tetraamminebis(isothiocyanato)chromium(1+), 8Cl.
Tetraamminedithiocyanatochromium(III)

[51266-66-1]

$[Cr(NCS)_2(NH_3)_4]^{\oplus}$

M 236.2 (ion)

cis-form [25125-68-2]

Thiocyanate: [19683-61-5].
Not isol.

trans-form

Perchlorate: [66916-72-1].
Synth. from *trans*-$[Cr(OH_2)_2(NH_3)_4](ClO_4)_3$ and ethanolic $[NH_4]NCS$ heated with a little $HClO_4$. Orange plates (0.01*M* $HCl/HClO_4$).

[52749-08-3]

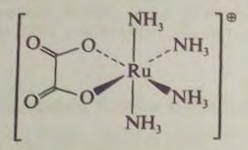
Oki, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 652 (*synth, uv*)
Kirk, A.D. *et al*, *Inorg. Chim. Acta*, 1978, **27**, 265 (*synth, uv*)
Kirk, A.D. *et al*, *J. Phys. Chem.*, 1980, **84**, 887 (*photochem*)

$C_2H_{12}N_4O_4Ru^{\oplus}$ IC-003364

Tetraammine(oxalato)ruthenium(*III*)(1+)

Tetraammine[ethanedioato(2−)-O,O′]ruthenium(III)(1+), *10Cl*

[45976-96-3]



M 257.2 (ion)
Approx. octahedral cation. Prepd. by treating $[Ru(NH_3)_5(OH)]^{2\oplus}$ with oxalic acid. Yellow salts.

Gleu, K. *et al*, *Z. Anorg. Allg. Chem.*, 1938, **237**, 335, 350 (*synth*)

$C_2H_{12}N_5ORuS^{\oplus}$ IC-003365

Tetraamminecarbonyl(thiocyanato-*S*)ruthenium(*II*)(1+)

$[Ru(NH_3)_4CO(SCN)]^{\oplus}$

M 255.2 (ion)
trans-Octahedral only reported isomer. Prepd. by treating Tetraammineaqua(carbonyl)ruthenium(*II*)(2+), IC-002668 with aq. NaSCN.

Thiocyanate: White salt.

Allen, A.D. *et al*, *Can. J. Chem.*, 1969, **47**, 1605 (*synth, ir*)

$C_2H_{12}N_6NiS_2$ IC-003366

Tetraamminebis(thiocyanato-*N*)nickel(*II*), 11Cl

[65138-17-2]

$Ni(NCS)_2(NH_3)_4$

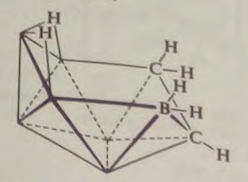
M 242.9
trans-Octahedral Ni. Sapphire-blue cryst. $\mu_{eff} = 3.28\mu_B$ (3.31).

[14409-26-8]

Grossman, N., *Z. Anorg. Allg. Chem.*, 1908, **58**, 265 (*synth*)
Asmussen, R.W. *et al*, *Acta Chem. Scand.*, 1957, **11**, 1097 (*magnetism*)
Porai-Koshits, M.A. *et al*, *Acta Crystallogr.*, 1957, **10**, 784 (*cryst struct*)

Porai-Koshits, M.A. *et al*, *Kristallografiya*, 1957, **2**, 371 (*cryst struct*)
Belova, V.I. *et al*, *Zh. Neorg. Khim.*, 1957, **2**, 1488; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1957, **2**, 63 (*magnetism*)
Hare, C.R. *et al*, *J. Chem. Phys.*, 1964, **40**, 792 (*uv-vis*)
Jona, E. *et al*, *J. Therm. Anal.*, 1975, **7**, 551 (*thermal dec*)

$C_2H_{13}B_7$
4,5-Dicarbanonaborane(13) IC-003367

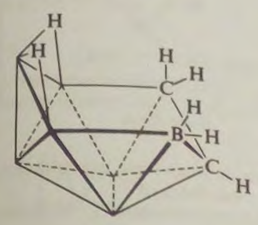


M 112.8
arachno-. Previously wrongly thought to be 2,6-$C_2B_7H_{11}$ or 2,5-$C_2B_8H_{11}$. Colourless cryst. Sol. aprotic solvs., dec. in alcohols or H_2O. Mp 90°.

Inorg. Synth., 1983, **22**, 237 (*synth, ir, pmr, B-11 nmr*)
Hermanek, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 927 (*synth, pmr, cmr, B-11 nmr, ms*)

$C_2H_{13}B_7$
6,7-Dicarbanonaborane(13) IC-003368
4,5-Dicarba-arachno-*nonaborane(13)*

[113678-30-1]

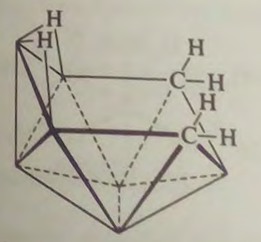


M 112.8
arachno-. Previously misassigned as *nido*-$C_2H_{11}B_7$. Sol. C_6H_6.

Rietz, R.R. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 1263 (*synth*)
Inorg. Synth., 1983, **22**, 237 (*synth*)
Hermanek, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 927 (*B-11 nmr, cmr, pmr, ms*)

$C_2H_{13}B_7$ IC-003369
6,8-Dicarbanonaborane(13), 11Cl, 10Cl, 9Cl, 8Cl

[17653-38-2]

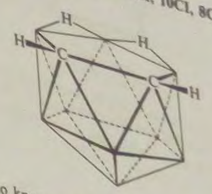


M 112.8
arachno-. Colourless solid. Sol. toluene, $CHCl_3$, CH_2Cl_2. Mp 61°.

Tebbe, F.N. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 869 (*synth, ir, pmr, B-11 nmr*)
Garrett, P.M. *et al*, *Inorg. Chem.*, 1969, **8**, 2008 (*synth*)
Base, K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1984, 299 (*synth*)

$C_2H_{13}B_9$
7,8-Dicarbaundecaborane(13), 11Cl, 10Cl, 8Cl IC-003370

[33806-57-4]

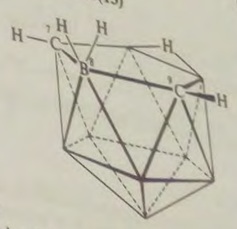


M 134.4
nido-. Also known as the 1,2-isomer in early lit. Colourless hygroscopic colourless cryst. Sol. C_6H_6, toluene, Et_2O. Mp 110° dec. pK_{a1} 2.95 ($MeOH/H_2O$ 1:3).

[34721-46-5]

Wiesboeck, R.A. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1642 (*synth, ir*)
Howe, D.V. *et al*, *Inorg. Chem.*, 1971, **10**, 2516 (*ir, B-11 nmr*)
Young, D.A.T. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, ir, pmr, B-11 nmr*)

$C_2H_{13}B_9$
7,9-Dicarbaundecaborane(13) IC-003371



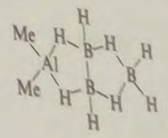
M 134.4
nido-. Colourless solid. Sol. C_6H_6.

Tebbe, F.N. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 4222 (*synth*)
Pretzer, W.R. *et al*, *Inorg. Chem.*, 1976, **15**, 1779 (*synth*)

$C_2H_{14}AlB_3$
Dimethyl[octahydrotriborato(1−)]aluminium IC-003372

Dimethylaluminium octahydrotriborate(1−). 2,2-Dimethyl-2-aluminatetraborane(8)

[12654-95-4]



M 97.5
Extremely sensitive to air and moisture. Thermally unstable, $t_{1/2} \sim 10$ min. at 20°/10-20 mm.

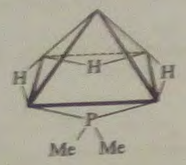
Borlin, J.-J. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 1387 (*synth, pmr, nmr*)
Dain, C.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 2465 (*synth, struct*)

IC-003373

$C_2H_{16}B_5P$

2,3-[μ-(Dimethylphosphino)]pentaborane(9), 9CI

[19624-24-9]



M 123.1
Proposed struct. shown. Synth. from Me_2PCl and LiB_5H_8 in Et_2O. Liq. Mp 17°. Bp 191° (est.).

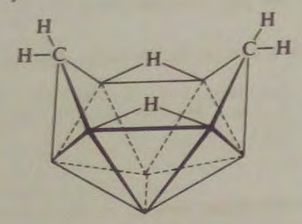
Burg, A.P. *et al, Inorg. Chem.*, 1968, **7**, 1021 (*synth, pmr, B-11, P-31 nmr, ir*)

IC-003374

$C_2H_{14}B_8$

6,9-Dicarbadecaborane(14), 9CI

[38670-58-5]



M 124.6
arachno-. Cryst. (C_6H_6 or column chromatog. C_6H_6/hexane). Sol. C_6H_6. Mp 146°.

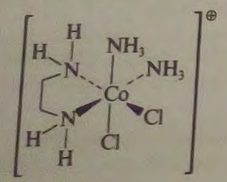
Stibr, B. *et al, Collect. Czech. Chem. Commun.*, 1974, **39**, 1805 (*ms, pmr, B-11 nmr, ir, uv*)
Janoušek, Z. *et al, Polyhedron*, 1985, **4**, 1797 (*ms, synth, B-11 nmr, pmr*)

IC-003375

$C_2H_{14}Cl_2CoN_4^{\oplus}$

Diamminedichloro(ethylenediamine)cobalt(*III*)(1+)

*Diamminedichloro(1,2-ethanediamine-*N,N′*)cobalt(1+), 9CI*



all-cis-form

M 223.9 (ion)

All-cis-form

Chloride: [14096-64-1].
$C_2H_{14}Cl_3CoN_4$ M 259.4
Violet solid.

trans-NH_3-form

Chloride: [14095-77-3].
Blue cryst. (MeOH aq.).

trans-Cl-form

Chloride: [36487-86-2].
Green cryst. (conc. HCl).

[20115-55-3]

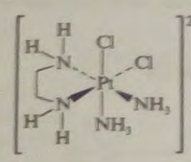
Bailar, J.C. *et al, J. Am. Chem. Soc.*, 1940, **62**, 105 (*synth*)
Hawkins, C.J. *et al, Aust. J. Chem.*, 1972, **25**, 273 (*synth, uv, cd*)
Tsuchiya, R. *et al, Bull. Chem. Soc. Jpn.*, 1972, **45**, 1065 (*isom*)

IC-003376

$C_2H_{14}Cl_2N_4Pt^{2\oplus}$

Diamminedichloro(ethylenediamine)platinum(*IV*)(2+), 8CI

[24229-03-6]



cis-form

M 360.1 (ion)
Octahedral, only the *cis*-form has been well studied. Acidity of NH_3 ligands studied.

cis-form [30904-77-9]

Chloride: [22615-79-8].
Sol. H_2O.
Nitrate: [73035-96-8].
Sol. H_2O.

[33270-76-7]

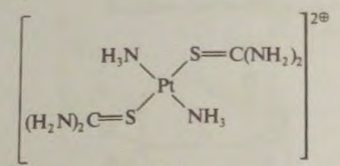
Adrianova, O.N. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1971, **16**, 586; 1980, **25**, 105 (*uv, ord, cd, acidity*)

IC-003377

$C_2H_{14}N_6PtS_2^{2\oplus}$

Diamminebis(thiourea-*S*)platinum(*II*)(2+), 11CI

[70497-80-2]



trans-form

M 381.3 (ion)
Probably known as *trans*-form but salts not widely known. Synth. from *trans*-form of Diamminedichloroplatinum(*II*), IC-016643 + thiourea. Synth. is test to distinguish *cis* from *trans*-$[Pt(NH_3)_2X_2]$, the former proceeding to Tetrakis(thiourea)platinum(*II*)(2+), IC-004393 (Kurnakov's test).

[14592-53-1, 28681-18-7]

Kurnakov, N.S., *J. Prakt. Chem.*, 1894, **50**, 483 (*synth*)
Woollins, J.D. *et al, Polyhedron*, 1983, **2**, 175 (*ir, pmr, cmr, Pt-195 nmr*)

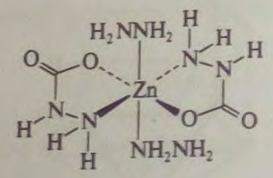
IC-003378

$C_2H_{14}N_8O_4Zn$

Bis(hydrazine-*N*)bis(hydrazinecarboxylato-N^2,O^1)zinc

Bis(carbazato)bis(hydrazine)zinc

[15293-39-7]



M 279.5
Octahedral at Zn with H-bonding between molecules. Cryst. (H_2O). Forms a monohydrate.

Bighardi, G. *et al, Gazz. Chim. Ital.*, 1965, **95**, 871 (*synth*)
Ferrari, A. *et al, Z. Kristallogr.*, 1965, **122**, 259 (*synth, cryst struct*)
Braibanti, A. *et al, Nature* (*London*), 1966, **211**, 1174 (*ir*)

Braibanti, A. *et al, Inorg. Chem.*, 1968, **7**, 1430 (*ir*)
Patil, K.C. *et al, Proc. Indian Acad. Sci., Chem. Sci.*, 1985, **95**, 345; 1986, **96**, 459 (*synth, thermal anal*)

IC-003379

$C_2H_{25}CoN_5O_4^{\oplus}$

Pentaammine(oxalato)cobalt(*III*)(1+)

Pentaammine[ethanedioato(2−)-O]cobalt(III)(1+), 9CI

[18443-73-7]

$[(H_3N)_5Co(OOCCOO)]^{\oplus}$

M 232.1 (ion)
Unusual monodentate C_2O_4.
Perchlorate: Solid. Sol. H_2O.

Saffir, P. *et al, J. Am. Chem. Soc.*, 1960, **82**, 13 (*synth*)
Vando, A.F. *et al, J. Am. Chem. Soc.*, 1972, **94**, 6655 (*uv, photochem*)

IC-003380

$C_2H_{15}N_5O_3Ru^{2\oplus}$

(Acetato-*O*)tetraammine(nitrosyl)ruthenium(2+), 9CI

$[Ru(NO)(OAc)(NH_3)_4]^{2\oplus}$

M 258.2 (ion)
trans-Octahedral. Prepd. by heating Tetraamminechloro(nitrosyl)ruthenium(2+), IC-016436 in acidic soln. with NaOAc. Sol. H_2O.
Diiodide: [36400-21-2].
Yellow salt. Ir ν_{NO} 1890 cm^{-1}.

[60182-92-6]

Schreiner, A.F. *et al, Inorg. Chem.*, 1972, **11**, 880 (*synth, ir, uv, mcd*)
Inorg. Synth., 1976, **16**, 13 (*synth*)

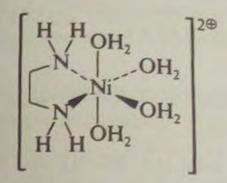
IC-003381

$C_2H_{16}N_2NiO_4^{2\oplus}$

Tetraaqua(ethylenediamine)nickel(*II*)(2+), 8CI

*Tetraaqua(1,2-ethanediamine-*N,N′*)nickel(II)(2+), 9CI*

[15615-30-2]



M 190.8 (ion)
Formed in solns. containing $Ni^{2\oplus}$, en and H_2O but more often converts to complexes with 2 or 3 en per Ni.
Dinitrate: [74009-08-8].
$C_2H_{16}N_4NiO_{10}$ M 314.8
Blue cylindrical cryst.
Sulfate, dihydrate: [70956-81-9].
$C_2H_{20}N_2NiO_{10}S$ M 322.9
Pale blue prisms. Monohydrate also known.

[43163-60-6]

McDougall, G.J. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 654.
Healy, P.C. *et al, Aust. J. Chem.*, 1984, **37**, 921.

IC-003382

$C_2H_{16}N_5O_4Rh^{2\oplus}$

Pentaammineoxalatorhodium(*III*)(2+)

$[Rh(NH_3)_5C_2O_4H]^{2\oplus}$

M 277.0 (ion)
Probably monodentate oxalate monoanion.
Perchlorate: [55046-61-2].

Colourless needles (aq. $HClO_4$). Ir $\nu_{C=O}$ 1781s, 1690sh, 1682s, 1660m, 1400s, 1230s cm^{-1}. Forms a double salt with $2NaClO_4$.
Weighardt, K. *et al, Z. Naturforsch., B*, 1974, **29**, 809 (*synth, ir*)

IC-003383

$C_2H_{16}N_{10}OS_2Zr$

Tetrakis(hydrazine-*N*)oxobis(thiocyanato-*N*)zirconium(*IV*), 11CI

Tetrakis(hydrazine)bis(isothiocyanato)oxozirconium(IV)

[81599-29-3]

$(H_2NNH_2)_2ZrO(NCS)_2$

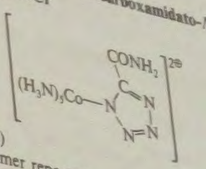
M 351.5
Synth. by reaction of hydrazine with $ZrO(NCS)_2$ in EtOH. Mp 210° dec.

Srivastava, A.K. *et al, Transition Met. Chem.*, 1982, **7**, 41 (*synth, ir, thermal dec*)

IC-003384

$C_2H_{17}CoN_{10}O^{2\oplus}$

Pentaammine(1*H*-tetrazole-5-carboxamidato-N^4)cobalt(*III*)(2+), 11CI



M 256.1 (ion)
Only one isomer reported.
Bis-tetrafluoroborate: [79717-55-8].

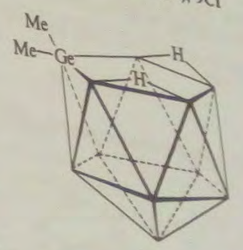
Balahura, R.J. *et al, Inorg. Chem.*, 1983, **22**, 3602 (*synth, pmr, cmr, redox kinetics*)

IC-003385

$C_2H_{18}B_{10}Ge$

7,7-Dimethyl-7-germaundecaborane(14), 9CI

[34514-72-2]

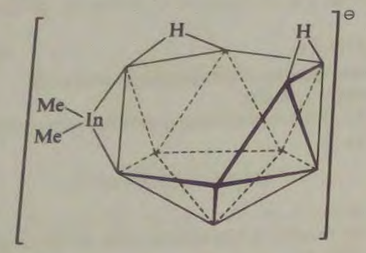


M 222.8
Proposed struct. shown. White solid. Mp 82-83°. Reasonably stable in air.

Loffredo, R.E. *et al, J. Am. Chem. Soc.*, 1971, **93**, 5587 (*synth, pmr, nmr, ms*)

$C_2H_{18}B_{10}In^{\ominus}$ IC-003386

[η^4-Dodecahydrodecaborato(2−)]dimethylindate(1−), 9CI



M 265.0 (ion)

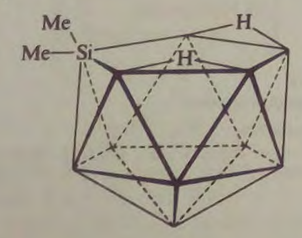
Dimethylindium(1+) salt: [55988-45-9].
$C_4H_{24}B_{10}In_2$ M 409.9
Pale-yellow cryst. Sol. Me_2CO, insol. C_6H_6.

Greenwood, N.N. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 299 (*synth, ir, B-11 nmr, pmr*)

$C_2H_{18}B_{10}Si$ IC-003387

7,7-Dimethyl-7-silaundecaborane(14), 10CI

[65554-56-5]



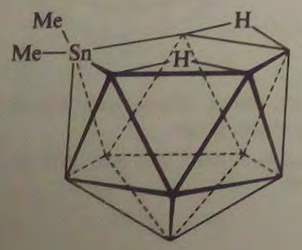
M 178.3
nido-. Synth. from $Na_2B_{10}H_{12}$ + Me_2SiCl_2 in C_6H_6 at 60°. Purif. by subl. Mp 59-60°.

Norman, A.D. *et al, Inorg. Nucl. Chem. Lett.*, 1977, **13**, 599 (*synth, pmr, B-11 nmr*)

$C_2H_{18}B_{10}Sn$ IC-003388

7,7-Dimethyl-7-stannaundecaborane(14), 9CI

[34514-71-1]

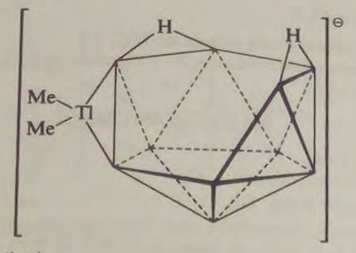


M 268.9
Proposed struct. shown. White solid. Mp 123-124°. Reasonably stable in air.

Loffredo, R.E. *et al, J. Am. Chem. Soc.*, 1971, **93**, 5587 (*synth, pmr, nmr, ms*)

$C_2H_{18}B_{10}Tl^{\ominus}$ IC-003389

[η^4-Dodecahydrodecaborato(2−)]dimethylthallate(1−), 9CI



M 354.6 (ion)

▷ Toxic.

Dimethylthallium(1+) salt:
$C_4H_{24}B_{10}Tl_2$ M 589.1
Large-waxy yellow plates. Sol. THF.

$MePh_3P$ salt: [58776-50-4].
Yellow cryst. (CH_2Cl_2, Et_2O at 0°).

Greenwood, N.N. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 299 (*synth, ir, B-11 nmr, pmr*)

$C_2H_{18}CoN_5O_2^{2\oplus}$ IC-003390

Acetatopentaamminecobalt(*III*)(2+)

$[Co(NH_3)_5OAc]^{2\oplus}$

M 203.1 (ion)
Prob. octahedral with monodentate acetate.

Dinitrate: Red cryst. Sl. sol. H_2O.

Inorg. Synth., 1953, **4**, 171 (*synth*)

$C_2H_{18}CoN_5O_5P^{\oplus}$ IC-003391

(Acetylphosphato)pentaamminecobalt(*III*)(1+)

[*Aceticphosphoricmonoanhydridato*(2−)-O]*pentaamminecobalt*(III)(1+)

[79737-95-4]

$[Co[OP(O)_2OAc](NH_3)_5]^{\oplus}$

M 282.1 (ion)

Perchlorate: Pink solid (aq. EtOH). Sol. H_2O.

Buckingham, D.A. *et al, Aust. J. Chem.*, 1981, **34**, 1769 (*synth, ir, uv, pmr, kinetics*)

$C_2H_{18}CoN_6^{3\oplus}$ IC-003392

(Acetonitrile)pentaamminecobalt(*III*)(3+), 10CI

[44819-13-8]

$[Co(NH_3)_5(NCCH_3)]^{3\oplus}$

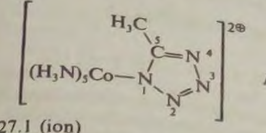
M 185.1 (ion)
Octahedral cation.

Diperchlorate, trifluoromethanesulfonate: [75522-58-6].
Yellow solid. Sol. H_2O.

Dixon, N.E. *et al, Inorg. Chem.*, 1981, **20**, 470 (*synth, uv, pmr*)

$C_2H_{18}CoN_9^{2\oplus}$ IC-003393

Pentaammine(5-methyl-1*H*-tetrazolato)cobalt(*III*)(2+), 11CI



N^1-bonded-form

M 227.1 (ion)
Ligand can coordinate through any N.

N^1-bonded-form

Diiodide, pentahydrate: Sol. H_2O, DMSO.
Diperchlorate: [84927-29-7].
Insol. H_2O.

N^2-bonded-form

Diiodide: [79899-68-6].
Sol. H_2O, DMSO.
Diperchlorate: [84927-31-1].
Insol. H_2O.

Ellis, W.R. *et al, Inorg. Chem.*, 1982, **21**, 835 (*synth, uv, pmr*)
Purcell, W.L., *Inorg. Chem.*, 1983, **22**, 1205 (*isom, kinetics*)

$C_2H_{18}CrN_5O_2^{2\oplus}$ IC-003394

(Acetato-*O*)pentaamminechromium(*III*)(2+), 10CI, 9CI

[27842-83-7]

$[Cr(OAc)(NH_3)_5]^{2\oplus}$

M 196.1 (ion)
Many analogous compds. known.

Diperchlorate: [22792-96-7].
Synth. from the dinitrate and aq. $NaClO_4$. Orange cryst.

Dinitrate: Synth. from $[Cr(OH_2)(NH_3)_5](NO_3)_3.NH_4NO_3$ and NaOAc in dimethylacetamide. Orange cryst. (aq. NH_4NO_3).

Zinato, E. *et al, Inorg. Chem.*, 1972, **11**, 1746 (*synth, aquation, uv*)
Jackman, L.M. *et al, Inorg. Chem.*, 1979, **18**, 1497 (*synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 780 (*rev*)

$C_2H_{18}IrN_6^{3\oplus}$ IC-003395

(Acetonitrile)pentaammineiridium(*III*)(3+), 10CI

Pentaammine(methyl cyanide)iridium(3+)

$[Ir(NH_3)_5(NCCH_3)]^{3\oplus}$

M 318.4 (ion)
Octahedral cation.

Triperchlorate: [73453-89-1].
White solid. Sol. H_2O.
▷ Potentially explosive.

Foust, R.D. *et al, Inorg. Chem.*, 1972, **11**, 899 (*synth, ir, uv*)
Talebinasab-sarvari, M. *et al, Inorg. Chem.*, 1980, **19**, 1835 (*synth, photochem, uv*)

$C_2H_{18}N_5O_2Rh^{2\oplus}$ IC-003396

Acetatopentaamminerhodium(*III*)(2+), 8CI

$[Rh(NH_3)_5OAc]^{2\oplus}$

M 247.1 (ion)

Diperchlorate: [14567-09-0].
White cryst. Sol. H_2O.
▷ Potentially explosive.

Monacelli, F. *et al, J. Inorg. Nucl. Chem.*, 1962, **24**, 1241; 1967, **29**, 1079 (*synth, uv, hydrol, kinetics*)

$C_2H_{18}N_5O_3Ru^{\oplus}$ IC-003397

(Acetato-*O*)pentaammineruthenium(*II*)(1+)

Pentaammine(ethanoato)ruthenium(II)

$[Ru(NH_3)_5OAc]^{\oplus}$

M 245.2 (ion)
Pseudo-octahedral; undergoes rapid aquation (rate constant $<5\ s^{-1}$). Prepd. by the electrochemical reduction of (Acetato-*O*)pentaammineruthenium(*III*)(2+), IC-003398. Only obsd. in soln. Sol. H_2O.

Stritar, J.A. *et al, Inorg. Chem.*, 1969, **8**, 2281 (*synth, electrochem, uv, aquation*)

$C_2H_{18}N_5O_3Ru^{2\oplus}$ IC-003398

(Acetato-*O*)pentaammineruthenium(*III*)(2+), 9CI

Pentaammineethanoatoruthenium(III)

[38744-91-1]

$[Ru(NH_3)_5(OAc)]^{2\oplus}$

M 245.2 (ion)
Readily reduced by common one-electron reducing agents; undergoes a wide range of anation and aquation reactions.

Diperchlorate: Prepd. either by heating $[Ru(NH_3)_5Cl]Cl_2$ with conc. NH_3, followed by glacial HOAc and $Na[ClO_4]$; or by oxidising the ruthenium(*II*) analogue. Yellow solid.
▷ Potentially explosive.

Stritar, J.A. *et al, Inorg. Chem.*, 1969, **8**, 2281 (*synth, uv, reactions*)
Lin, S.-W. *et al, Inorg. Chim. Acta*, 1971, **5**, 290 (*synth, uv*)
Ohyoshi, A. *et al, Bull. Chem. Soc. Jpn.*, 1972, **45**, 2121; 1973, **46**, 2431 (*reactions*)
Ohkubo, K. *et al, Bull. Chem. Soc. Jpn.*, 1973, **46**, 2651; 1975, **48**, 774 (*reactions*)
Ohyoshi, A. *et al, Chem. Lett.*, 1973, 737 (*electrochem*)

$C_2H_{18}N_6Ru^{2\oplus}$ IC-003399

(Acetonitrile)pentaammineruthenium(*II*)(2+), 9CI

Pentaammine(ethanenitrile)ruthenium(II)

[26540-31-8]

$[Ru(NH_3)_5N{\equiv}CCH_3]^{2\oplus}$

M 227.2 (ion)
Octahedral. Prepd. by treatment of Pentaammine(aqua) ruthenium(*II*)(2+), IC-019980 with MeCN or by treating Hexaammineruthenium(*III*)(3+), IC-020001 with $MeCHO/OH^{\ominus}$, followed by O_2 or H_2O_2. Sol. H_2O.

Dichloride:
$C_2H_{18}Cl_2N_6Ru$ M 298.1
Yellow. Ir ν_{CN} 2237 cm^{-1} (nujol).

Dibromide: Yellow salt. Ir ν_{CN} 2238 cm^{-1} (nujol).

Diiodide:
$C_2H_{18}I_2N_6Ru$ M 481.0
Yellow-green salt. Ir ν_{CN} 2239 cm^{-1} (nujol).

Bis-tetrafluoroborate: Yellow salt. Ir ν_{CN} 2253 cm^{-1} (nujol).

Bis-hexafluorophosphate: Yellow salt. Ir ν_{CN} 2277 cm^{-1} (nujol).

Clarke, R.E. *et al, Inorg. Chem.*, 1970, **9**, 227 (*synth, ir, uv, reaction*)
Chatt, J. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 3168 (*synth, ir, pmr*)
Allen, R.J. *et al, Inorg. Chem.*, 1972, **11**, 679 (*formn*)
Foust, R.D. *et al, J. Am. Chem. Soc.*, 1972, **94**, 5686 (*pmr*)
Hintze, R.E. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2664 (*reaction, photochem*)

Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*electrochem*)
Guengerich, C.P. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 3298 (*synth, ir, uv*)

$C_2H_{18}N_6Ru^{3\oplus}$ IC-003400

(Acetonitrile)pentaammineruthenium(*III*)(3+), 9CI

Pentaammine(ethanenitrile)ruthenium(III)(*3+*)

[44819-54-7]

$[Ru(NH_3)_5(NCCH_3)]^{3\oplus}$

M 227.2 (ion)
Usually only generated in soln. Prepd. by *in situ* oxidation of the ruthenium(*II*) analogue. Sol. H_2O.

Tribromide: Studied by X-ray photoelectron spectrosc.

Ford, P.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 1109 (*synth*)
Clarke, R.E. *et al*, *Inorg. Chem.*, 1970, **9**, 227 (*synth, uv, ir*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*electrochem*)
Battistoni, C. *et al*, *Inorg. Chim. Acta*, 1977, **21**, L25 (*pe*)

$C_2H_{19}CoN_9^{3\oplus}$ IC-003401

Pentaammine(*N*-cyanoguanidine)cobalt(*III*)(3+), 8CI

[31253-58-4]

$[Co[N{\equiv}CN{=}C(NH_2)_2](NH_3)_5]^{3\oplus}$

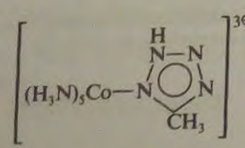
M 228.1 (ion)
Octahedral geometry. Kinetics of the Cr(*II*) reduction for this complex have been studied.

Triperchlorate: Solid. Sol. DMSO.
▷ Potentially explosive.

Balahura, R.J. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 625 (*synth, ir, uv, pmr, kinetics*)

$C_2H_{19}CoN_9^{3\oplus}$ IC-003402

Pentaammine(5-methyl-1*H*-tetrazole-N^1)cobalt(*III*)(3+), 11Cl



M 228.1 (ion)
Prepd. as an intermed. in the acid dissoc. of $[(NH_3)_5Co(N_4CCH_3)](ClO_4)_2$ in aq. $HClO_4$.

Triperchlorate: Present in soln., not isol.

[84927-27-5, 84943-93-1]

Ellis, W.R. *et al*, *Inorg. Chem.*, 1982, **21**, 835 (*synth*)
Purcell, W.L. *et al*, *Inorg. Chem.*, 1983, **22**, 1205 (*synth, kinetics*)

$C_2H_{21}CoN_5OS^{3\oplus}$ IC-003403

Pentaammine(dimethyl sulfoxide)cobalt(*III*)(3+)

Pentaammine[sulfinylbis[methane]-O]cobalt(3+), 10Cl

[44915-85-7]

$[Co(NH_3)_5O{=}SMe_2]^{3\oplus}$

M 222.2 (ion)

Tris-trifluoromethanesulfonate: [75522-60-0].
Red violet cryst. Sol. H_2O, DMSO.

Dixon, N.E. *et al*, *Inorg. Chem.*, 1981, **20**, 470 (*synth, uv, pmr, kinetics*)

$C_2H_{21}N_5ORuS^{2\oplus}$ IC-003404

Pentaammine(dimethyl sulfoxide-*S*)ruthenium(*II*)(2+)

Pentammine[sulfinylbis[methane]-S]ruthenium(2+), 9Cl

$[Ru(NH_3)_5S(O)Me_2]^{2\oplus}$

M 264.3 (ion)
Pseudo-octahedral with Ru—S 218.8; S—O 152.7 Ru—$N_{trans toS}$ 220.9 Ru—$N_{trans toN}$ 216.9 pm. Prepd. by treating aq. Pentaammine(dinitrogen)ruthenium(*II*)(2+), IC-019958 or Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with DMSO. Sol. H_2O, DMSO.

Diiodide: [17457-16-8].
$C_2H_{21}I_2N_5ORuS$ M 518.1
Yellow cryst.

Bis-tetrafluoroborate: Yellow cryst.

Bis-hexafluorophosphate: [17457-17-9].
Yellow cryst.

Allen, A.D. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 5595 (*synth, ir*)
Senoff, C.V. *et al*, *Can. J. Chem.*, 1971, **49**, 3585 (*ir*)
March, F.C. *et al*, *Can. J. Chem.*, 1971, **49**, 3590 (*cryst struct*)
Kuehn, C.G. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 689 (*synth, electrochem*)

$C_2H_{21}N_5RuS^{2\oplus}$ IC-003405

Pentaammine(dimethyl sulfide)ruthenium(*II*)(2+)

Pentaammine[thiobis[methane]]ruthenium(2+), 9Cl

[58619-10-6]

$[Ru(NH_3)_5SMe_2]^{2\oplus}$

M 248.3 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with SMe_2. Sol. H_2O.

Dichloride: Yellow salt.
Diperchlorate: Yellow salt.
Bis-tetrafluoroborate: Yellow salt.
Bis-hexafluorophosphate: Yellow salt.

Kuehn, C.G. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 689 (*synth, electrochem, uv, ir, raman, pmr*)
Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 1168 (*synth, uv, electrochem*)

$C_2H_{21}N_5RuS^{2\oplus}$ IC-003406

Pentaammine(ethanethiol)ruthenium(*II*)(2+), 9Cl

$[Ru(NH_3)_5S(H)Et]^{2\oplus}$

M 248.3 (ion)
Pseudo-octahedral. Prepd. by heating Pentaammine(aqua) ruthenium(*II*)(2+), IC-019980 with ethanethiol. Sol. H_2O. pK_a 9.2.

Bis-tetrafluoroborate: [58619-15-1].
Yellow cryst.

Kuehn, C.G. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 689 (*synth, ir, uv, pmr, raman, electrochem*)

$C_2H_{21}N_5RuS^{3\oplus}$ IC-003407

Pentaammine(dimethyl sulfide)ruthenium(*III*)(3+)

Pentaammine[thiobis[methane]]ruthenium(3+), 9Cl

[69204-65-5]

$[Ru(NH_3)_5SMe_2]^{3\oplus}$

M 248.3 (ion)

Prepd. by the chemical (Ce(*IV*), O_2 or H_2O_2) or electrochemical oxidation of Pentaammine(dimethyl sulfide)ruthenium(*II*)(2+), IC-003405. Orange aq. soln.; not isol. Sol. H_2O.

Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 1168, 2212 (*synth, uv, electrochem*)

$C_2H_{21}N_5RuSe^{2\oplus}$ IC-003408

Pentaammine(dimethyl selenide)ruthenium(*II*)(2+)

Pentaammine[selenobis[methane]]ruthenium(2+), 10Cl

[69204-61-1]

$[Ru(NH_3)_5SeMe_2]^{2\oplus}$

M 295.2 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with $SeMe_2$. Sol. H_2O.

Bis-hexafluorophosphate: [69204-62-2].
Yellow cryst.

Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 1168 (*synth, uv, electrochem*)

$C_2H_{21}N_5RuSe^{3\oplus}$ IC-003409

Pentaammine(dimethyl selenide)ruthenium(*III*)(3+)

Pentaammine[selenobis[methane]]ruthenium(3+), 10Cl

[69204-64-4]

$[Ru(NH_3)_5SMe_2]^{3\oplus}$

M 295.2 (ion)
Prepd. by the chemical (Ce(*IV*), O_2 or H_2O_2) or electrochemical oxidation of Pentaammine(dimethyl selenide)ruthenium(*II*)(2+), IC-003408. Not isol. as a solid salt. Sol. H_2O.

Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 1168 (*synth, uv, electrochem*)

$C_2H_{21}N_5RuTe^{2\oplus}$ IC-003410

Pentaammine(dimethyl telluride)ruthenium(*II*)(2+)

Pentaammine[tellurobis(methane)]ruthenium(2+), 10Cl

[69204-59-7]

$[Ru(NH_3)_5TeMe_2]^{2\oplus}$

M 343.8 (ion)
Prep. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with $TeMe_2$. Sol. H_2O.

Bis-hexafluorophosphate: [69204-60-0].
Yellow salt.

Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 1168 (*synth, uv, electrochem*)

$C_2H_{21}N_5RuTe^{3\oplus}$ IC-003411

Pentaammine(dimethyl telluride)ruthenium(*III*)(3+)

Pentaammine[tellurobis[methane]]ruthenium(3+), 10Cl

[69204-63-3]

$[Ru(NH_3)_5TeMe_2]^{3\oplus}$

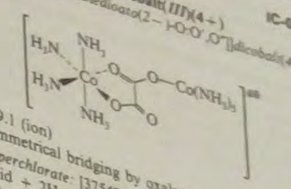
M 343.8 (ion)
Prepd. by the chemical (Ce(*IV*), O_2 or H_2O_2) or electrochemical oxidation of Pentaammine(dimethyl telluride)ruthenium(*II*)(2+), IC-003410. Not isol. as a solid salt. Sol. H_2O.

Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 1168 (*synth, uv, electrochem*)

$C_2H_2Co_2N_3O_4^{4\oplus}$ IC-003412

Nonaammine-μ-oxalatodicobalt(*III*)(4+)

Nonaammine[μ-[ethanedioato(2−)-O:O′,O″]]dicobalt(4+), 9Cl



M 359.1 (ion)
Unsymmetrical bridging by oxalate.

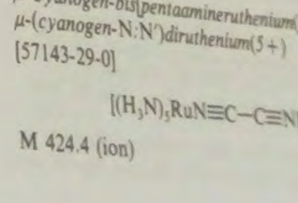
Tetraperchlorate: [37540-71-9].
Solid + $2H_2O$. Sol. H_2O.
▷ Potentially explosive.

Scott, K.L. *et al*, *Inorg. Chem.*, 1973, **12**, 655 (*synth, ir, uv*)

$C_2H_{29}Co_2N_3O_5^{4\oplus}$ IC-003413

Nonaammineaqua-μ-oxalatodicobalt(*III*)(4+)

Nonaammineaqua[μ-[ethanedioato(2−)-O:O′]]dicobalt(III)(4+), 9Cl



M 377.1 (ion)
Prob. struct. shown.

Tetrabromide: [37523-51-6].
Solid + $2H_2O$. Sol. H_2O.

Tetraperchlorate: [37540-73-1].
Red cryst. + $1H_2O$.
▷ Potentially explosive.

Scott, K.L. *et al*, *Inorg. Chem.*, 1973, **12**, 655 (*synth, ir, uv*)

$C_2H_{30}N_{12}Ru_2^{4\oplus}$ IC-003414

Decaammine[μ-(ethanedinitrile-*N*:*N*′)]diruthenium(4+), 10Cl

μ-Cyanogen-bis[pentaammineruthenium(II)*]. Decaammine-μ-(cyanogen-N:N′)diruthenium(4+)*

[73969-40-1]

$[(H_3N)_5RuN{\equiv}C{-}C{\equiv}NRu(NH_3)_5]^{4\oplus}$

M 424.4 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with cyanogen in H_2O. Sol. H_2O, DMF, DMSO, MeCN.

Tetrabromide: Solid.
Tetrakis-(4-methylbenzenesulfonate): Solid.

Tom, G.M. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 5310 (*synth, uv, electrochem, ir*)

$C_2H_{30}N_{12}Ru_2^{5\oplus}$ IC-003415

Decaammine[μ-(ethanedinitrile-*N*:*N*′)]diruthenium(5+), 10Cl

μ-Cyanogen-bis[pentaammineruthenium(III)*]. Decaammine-μ-(cyanogen-N:N′)diruthenium(5+)*

[57143-29-0]

$[(H_3N)_5RuN{\equiv}C{-}C{\equiv}NRu(NH_3)_5]^{5\oplus}$

M 424.4 (ion)

Class III mixed-valence ion. Prepd. by oxidising Decaammine[μ-(ethanedinitrile-*N*:*N'*)]diruthenium(4+), IC-003414 in DMF with $[Fe(bipy)_3]^{3\ominus}$ or Br_2. Not isol. pure in the solid state. Sol. H_2O, DMF, MeCN, DMSO.

Tom, G.M. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 5310 (*synth, uv, nir, ir, hydration*)
Battistoni, C. *et al*, *Inorg. Chim. Acta*, 1977, **21**, L25 (*pe*)
Taube, H., *Ann. N.Y. Acad. Sci.*, 1978, **313**, 481 (*electron transfer*)
Tanner, M. *et al*, *Inorg. Chem.*, 1981, **20**, 2348 (*vibronic coupling*)
Richardson, D.E. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 40 (*nir*)
Creutz, C., *Prog. Inorg. Chem.*, 1983, **30**, 1 (*electron transfer*)

IC-003416

$C_2HfN_2OS_2$

Oxobis(thiocyanato-*S*)hafnium(*IV*), 11CI

[72017-88-0]

$(NCS)_2Hf{=}O$

M 310.6

Formed by thermal dec. of Bis(cycloheptyldithiocarbamato-*S*,*S'*)oxohafnium(*IV*), IC-009415.

Pandey, O.P. *et al*, *J. Therm. Anal.*, 1986, **31**, 387 (*synth*)

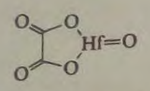
IC-003417

C_2HfO_5

Oxalatooxohafnium(*IV*)

[*Ethanedioato*(2−)-O,O']*oxohafnium*(IV), *11CI*

[12188-71-5]



M 282.5

Synth. by dissolving $HfCl_4$ in ice-cold H_2O then adding aq. $H_2C_2O_4$. Involved in methods of separating Zr and Hf. White solid. Insol. H_2O, Me_2CO.

3.5 Hydrate: [99043-09-1].

Pakajoff, Sw., *Mikrochim. Acta*, 1966, 751 (*rev, use*)
Sharma, A.K. *et al*, *Thermochim. Acta*, 1985, **83**, 347 (*rev*)
Mittal, S. *et al*, *Thermochim. Acta*, 1985, **89**, 195 (*synth, thermal dec*)

IC-003418

C_2HgN_2

Mercury(*II*) cyanide ($Hg(CN)_2$)

Mercuric cyanide

[592-04-1]

$Hg(CN)_2$

M 252.6

Low P-form comprises zig-zag chains of $Hg(CN)_2$, connected by Hg.....N contacts. Synth. from HgO and HCN. Glycosidation catalyst. Two forms: greyish cryst. (low P-form). Dark brown solid (high P-form $>6 \times 10^4$ atm.). Sol. H_2O (9.3 g per 100 cm^3 at 14°); sol. EtOH (8.2 g per 100 cm^3 at 19.5°). Dec. to Hg and $(CN)_2$ at 320° (440°). Weak electrolyte.

▷ OW1515000.

Hvoslef, J., *Acta Chem. Scand.*, 1958, **12**, 1568 (*cryst struct*)
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, **2**, 1121 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1197.
Ikeda, R. *et al*, *J. Phys. Chem.*, 1968, **72**, 2982 (*N-14 nqr*)
Seccombe, R.C. *et al*, *J. Organomet. Chem.*, 1969, **18**, 243 (*nd*)
Mason, W.R., *J. Am. Chem. Soc.*, 1973, **95**, 3573 (*uv-vis*)
Dehnicke, G. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1974, **78**, 1010 (*ir*)
Burroughs, P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1974, 921 (*pe*)
Goggin, P.L. *et al*, *J. Chem. Res. (S)*, 1979, 194 (*cmr, Hg-199 nmr*)
Sano, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 2023 (*pe*)
Sano, M. *et al*, *Inorg. Chem.*, 1982, **21**, 2521 (*cmr, N-15 nmr*)
Albright, M.T. *et al*, *J. Organomet. Chem.*, 1983, **259**, 37 (*Hg-199 nmr*)
Adams, D.M. *et al*, *J. Phys. C*, 1983, **16**, 3349 (*raman, phase trans*)
Wong, P.T.T., *J. Chem. Phys.*, 1984, **80**, 5937 (*raman, cryst struct*)
Dangerous Prop. Ind. Mater. Rep., 1986, **6**, 68 (*haz*)
Grishin, Yu.K. *et al*, *Zh. Strukt. Khim.*, 1987, **28**, 45 (*Hg-199 nmr*)

IC-003419

$C_2HgN_2O_2$

Mercury(*II*) cyanate

$Hg(OCN)_2$

M 284.6

Light-sensitive cryst. (Et_2O). Sol. H_2O (7.5 g per 100 cm^3 at 20°), MeOH, EtOH, Me_2CO, MeCN; spar. sol. $CHCl_3$, Et_2O.

Birckenbach, L. *et al*, *Ber.*, 1935, **68**, 895.
Goubeau, J., *Ber.*, 1935, **68**, 912 (*raman*)
Söderbäck, E., *Acta Chem. Scand.*, 1957, **11**, 1622 (*synth*)
Rao, C.N.R. *et al*, *J. Sci. Ind. Res.*, 1959, **186**, 169 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1227.

IC-003420

$C_2HgN_2O_2$

Mercury(*II*) fulminate

$Hg(ONC)_2$

M 284.6

From $Hg(NO_3)_2$ and EtOH, aldehydes or acetals. Detonator. White solid when pure. Poorly sol. org. solvs.; sl. sol. cold H_2O.

▷ Detonator.

Wöhler, L. *et al*, *Z. Anorg. Allg. Chem.*, 1930, **43**, 59.
Miles, D., *J. Chem. Soc.*, 1931, 2532 (*struct*)
Boldyrev, V.V., *Zh. Fiz. Khim.*, 1956, **30**, 1088.
Singh, K., *J. Chem. Soc.*, 1959, 459 (*ir, uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1229 (*rev, bibl*)

IC-003421

$C_2HgN_2S_2$

Mercury(*II*) thiocyanate

NCSHgSCN

M 316.7

Synth. from $Hg(NO_3)_2$ and K(SCN). Light-sensitive colourless needles (EtOH). Spar. sol. H_2O (0.07 g per 100 cm^3 at 25°); greater sol. EtOH. K_{sp} 3.0×10^{-20} at 25°. Swells up to an extraordinary bulk when heated (Pharoah's serpent).

Gallais, F. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1946, **223**, 722, 790 (*stability const*)
Tanaka, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1962, **35**, 124 (*stability const*)
Tramer, A. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1962, **59**, 232 (*ir, raman*)
Larsson, R. *et al*, *Acta Chem. Scand.*, 1965, **19**, 47 (*ir*)
Puff, H. *et al*, *Acta Crystallogr.*, 1965, **18**, 299 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1249.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1063 (*synth*)

IC-003422

$C_2HgN_2Se_2$

Mercury(*II*) selenocyanate

Bis(selenocyanato)mercury

$Hg(SeCN)_2$

M 410.5

From KSeCN and $Hg(NO_3)_2$ in $(NH_4)OAc$ buffer. Cream powder. Insol. cold H_2O; dec. in hot H_2O.

Aynsley, E.E. *et al*, *J. Chem. Soc.*, 1965, 2395 (*synth, ir*)
Kharitonov, Yu.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 1803 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1262 (*rev, bibl*)

$C_2HgN_5^{\ominus}$

(Azido)bis(cyano-*N*)mercurate(1−) IC-003423

Azidodiisocyanomercurate(1−)

$[Hg(NC)_2N_3]^{\ominus}$

M 294.6 (ion)

Na salt: [73596-72-2].
Cryst. + $2H_2O$.
K salt: [73596-76-6].
Cryst.

Thiele, G. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **461**, 109 (*ir, raman, synth, cryst struct*)

$C_2HgN_5O_2^{\ominus}$

Azidobis(fulminato)mercurate(1−) IC-003424

$[Hg(N_3)(ONC)_2]^{\ominus}$

M 326.6 (ion)

▷ Prob. explosive.

Ph_4As salt: [18582-99-5].
Solid.

Beck, W. *et al*, *Chem. Ber.*, 1967, **100**, 2335 (*synth, ir*)

C_2HgO_4

Mercury oxalate (HgC_2O_4) IC-003425

Mercury(2+) ethanedioate (1:1). Mercuric oxalate

[3444-13-1]

$Hg(C_2O_4)$

M 288.6

Precipitates on addition of $Hg(OAc)_2$ to oxalic acid in water. Unstable powder. Darkens rapidly in light.

▷ Detonates on impact when dry.

Prout, E.G. *et al*, *Trans. Faraday Soc.*, 1947, **43**, 148 (*synth, thermal dec*)

$C_2Hg_2N_2$

IC-003426

Mercury(*I*) cyanide($Hg_2(CN)_2$)

[37020-93-2]

$Hg_2(CN)_2$

M 453.2

Attempts to synthesise $Hg_2(CN)_2$ lead only to $Hg(CN)_2$ and Hg. Produced as a transient species by radiolysis of $Hg(CN)_2$. λ_{max} 285 nm.

Fujita, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 3067 (*formn*)
Jungbluth, H. *et al*, *J. Phys. Chem.*, 1976, **80**, 1049 (*formn*)

$C_2Hg_2N_2O$

IC-003427

Mercury(*II*) cyanide oxide ($Hg_2(CN)_2O$)

Basic mercury cyanide. Mercuric oxycyanide

[1335-31-5]

$Hg_2(CN)_2O$

M 469.2

Prepd. from $Hg(CN)_2$ + HgO. Formerly used as a topical antiseptic when mixed with mercuric cyanide to eliminate the danger of explosion. White cryst. (H_2O). Sol. H_2O.

▷ V. poisonous. Explosive, sensitive to impact and heat. OW1530000.

Jones, A.J., *Pharm. J.*, 1920, **105**, 87 (*synth, props*)
Scavnicar, S., *Z. Kristallogr.*, 1963, **118**, 248 (*cryst struct*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2198.

$C_2Hg_2N_2O_2$

Mercury(*I*) cyanate IC-003428

Dimercury(2+) dicyanate. Bis(cyanato)dimercury

M 485.2 NCOHgHgOCN

Synth. from $Hg_2(NO_3)_2$ + NaOCN in dil. aq. HNO_3. Disproportionates in hot H_2O to Hg and $Hg(OCN)_2$.

Söderbäck, E., *Acta Chem. Scand.*, 1957, **11**, 1622 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1227.

$C_2Hg_2N_2S_2$

Mercury(*I*) thiocyanate IC-003429

Bis(thiocyanato)dimercury

NCSHgHgSCN

M 517.3

Synth. from $Hg_2(NO_3)_2$ and K(SCN) in dil. soln. Colourless light-sensitive powder. Unstable: dec. to $Hg(SCN)_2$ and Hg. Spar. sol. H_2O (0.03 g per 100 cm^3 at 25°).

Burriel, F. *et al*, *An. R. Soc. Esp. Fis. Quim., Ser. B*, 1950, **46**, 169, 577 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1248 (*rev, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1063 (*synth*)

$C_2IN_2^{\ominus}$

Bis(cyano-C)iodate(1−) IC-003430

$[NClCN]^{\ominus}$

M 178.9 (ion)

I—C 229.8, N—C 112.9 pm; angle NCI 178.6° (K salt).

K salt: [88770-08-5].
C_2IKN_2 M 218.0
Formed from KCN + I_2. Monoclinic cryst. Layer lattice struct.

Tebbe, K.F. *et al*, *Z. Naturforsch., B*, 1988, **43**, 149 (*synth, cryst struct*)

$C_2I_2IrO_2^{\ominus}$

Dicarbonyldiiodoiridate(1−), 10CI IC-003431

As Dibromodicarbonyliridate(1−), IC-002834 with X = I

M 502.0 (ion)

***cis*-form**

Ph_4As salt: [29629-79-6].
Yellow cryst. Mp 158°. Ir ν_{CO} 2049, 1973 cm^{-1} ($MeNO_2$).

Malatesta, L. *et al*, *J. Chem. Soc.*, 1964, 961 (*synth*)
Forster, D. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 433 (*synth, ir*)

Forster, D., *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 221 (*synth, ir*)
Piraino, P. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 1237 (*synth, ir*)
Forster, D., *J. Chem. Soc., Dalton Trans.*, 1979, 1639 (*ir*)

IC-003432

$C_2I_2IrO_2$
Dicarbonyldiiodoiridium

$[Ir(CO)_2I_2]_n$

M 502.0
Polymeric, *n* unknown. Bright-yellow cryst. Subl. 150° in a stream of CO.

Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1941, **246**, 138 (*synth*)

IC-003433

$C_2I_2N_2P_2$
Hypodiphosphorous dicyanide diiodide, 10CI
P,P'-Dicyano-P,P'-diiododiphosphine. 1,2-Dicyano-1,2-diiododiphosphane. 1,2-Dicyano-1,2-diiododiphosphorus(III)
[79988-15-1]

NC(I)P—P(I)CN

M 367.7
Obt. only in soln. with other cyanodiphosphines.

Dillon, K.B. *et al, Inorg. Nucl. Chem. Lett.*, 1981, **17**, 201 (*synth, P-31 nmr*)

IC-003434

$C_2I_2N_2P_2$
Hypodiphosphorous dicyanide diiodide, 10CI
P,P-Dicyano-P',P'-diiododiphosphine. 1,1-Dicyano-2,2-diiododiphosphane. 1,1-Dicyano-2,2-diiododiphosphorus(III)
[79988-14-0]

$(NC)_2P—PI_2$

M 367.7
Obt. as mixt. with symmetrical isomer Hypodiphosphorous dicyanide diiodide, IC-003433. Synth. from P_2I_4 + AgCN.

Dillon, K.B. *et al, Inorg. Nucl. Chem. Lett.*, 1981, **17**, 201 (*synth, P-31 nmr*)

IC-003435

$C_2I_2O_2Os$
Dicarbonyldiiodoosmium
Osmium dicarbonyl diiodide

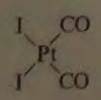
$[I_2Os(CO)_2]_n$

M 500.0
Polymeric. Yellow cryst. Ir ν_{CO} 2119, 2045, 1988 cm^{-1} (nujol).

Hales, L.A.W. *et al, J. Chem. Soc. A*, 1967, 1932.

IC-003436

$C_2I_2O_2Pt$
Dicarbonyldiiodoplatinum
Diiodoplatinum dicarbonyl. Dicarbonylplatinum diiodide
[77828-68-3]



M 504.9
trans-Form rapidly converts to *cis* isomer in soln.

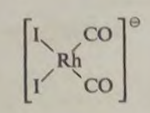
cis-form
Not cryst. Subl. from 40°, dec. at 150°. Dec. in C_6H_6 to give $Pt_2I_4(CO)_2$. Ir ν_{CO} 2147 cm^{-1} (toluene).

trans-form
Red. Ir ν_{CO} 2121 cm^{-1} (toluene).

Malatesta, L. *et al, Gazz. Chim. Ital.*, 1960, **90**, 1505 (*synth*)
Andreini, B.P. *et al, J. Organomet. Chem.*, 1988, **354**, 357 (*synth, cmr, ir*)

IC-003437

$C_2I_2O_2Rh^{\ominus}$
Dicarbonyldiiodorhodate(1−), 10CI
Diiododicarbonylrhodate(1−)
[38255-39-9]



M 412.7 (ion)
Catalyst for the carbonylation of alcohols, especially MeOH to AcOH.

cis-form [44516-57-6]
Tetrabutylammonium salt: [30192-00-8].
Mustard-yellow cryst. Mp 78° dec. Ir ν_{CO} 2052, 1985 cm^{-1} (nujol). Cannot be recryst., loses CO rapidly in soln.
Ph_4As salt: [13986-81-7].
Light-brown cryst. Mp 121° dec. Ir ν_{CO} 2043, 1967 cm^{-1} (nujol). Cannot be recryst., loses CO rapidly in soln.

Vallarino, L.M., *Inorg. Chem.*, 1965, **4**, 161 (*synth, ir*)
Griffith, W.P. *et al, J. Chem. Soc. A*, 1970, 2788 (*ir*)
Roth, J.F. *et al, Chem. Technol.*, 1971, 600 (*use*)
Forster, D., *J. Am. Chem. Soc.*, 1976, **98**, 846 (*use, ir*)
Hjortkjaer, J. *et al, J. Chem. Soc., Perkin Trans. 2*, 1978, 763 (*use*)
Baker, E.C. *et al, J. Am. Chem. Soc.*, 1980, **102**, 1020 (*use*)

IC-003438

$C_2I_2O_2Ru$
Dicarbonyldiiodoruthenium
[16369-42-9]

$Ru(CO)_2I_2$

M 410.9
Monomeric and polymeric forms known.
Monomer: [28986-72-3].
Yellow.
Polymer: [29088-68-4].
Dark orange-tan solid.

Colton, R. *et al, Aust. J. Chem.*, 1967, **20**, 1283 (*synth, ir*)
Abrahamson, H.B. *et al, J. Am. Chem. Soc.*, 1979, **101**, 4123 (*synth*)

IC-003439

$C_2I_4IrO_2^{\ominus}$
Dicarbonyltetraiodoiridate(1−)
Tetraiododicarbonyliridate(1−)
As Tetrabromodicarbonyliridate(1−), IC-002840 with

X = I

M 755.8 (ion)
Formed during the iridium-catalysed carbonylation of methanol.

cis-form
K salt:
$C_2I_4IrKO_2$ M 794.9
Red cryst.
Cs salt: [30191-84-5].
$C_2CsI_4IrO_2$ M 888.7
Cryst. (Me_2CO/pet. ether).
Benzyltrimethylammonium salt: [38268-47-2].

Red cryst.
Ph_4As salt: [30191-83-4].
Red cryst. Mp 210°. Ir ν_{CO} 2109, 2074 cm^{-1} (nujol).

Malatesta, L. *et al, J. Chem. Soc.*, 1964, 961 (*synth, ir*)
Cleare, M.J. *et al, J. Chem. Soc. A*, 1970, 2788 (*synth, ir*)
Forster, D., *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 221 (*synth*)
Malatesta, L. *et al, J. Organomet. Chem.*, 1974, **73**, 265 (*synth*)
Forster, D., *J. Chem. Soc., Dalton Trans.*, 1979, 1639 (*ir, use*)

$C_2I_4O_2Os^{2\ominus}$
Dicarbonyltetraiodoosmate(2−), 9CI **IC-003440**
As Tetrabromodicarbonylosmate(1−), IC-002841 with

X = I, *n* = 2

M 753.8 (ion)

trans-form
Di-Cs salt: [55399-57-0].
$C_2Cs_2I_4O_2Os$ M 1019.6
Yellow-green. Insol. org. solvs., mod. sol. H_2O.
Bis-tetrabutylammonium salt: Yellow-green needles. Sol. Me_2CO, $CHCl_3$, CH_2Cl_2, spar. sol. EtOH.

Preetz, W. *et al, J. Organomet. Chem.*, 1975, **86**, 397 (*synth, ir, uv*)

IC-003441

$C_2I_4O_2Os^{\ominus}$
Dicarbonyltetraiodoosmate(1−), 9CI
As Tetrabromodicarbonylosmate(1−), IC-002841 with

X = I, *n* = 1

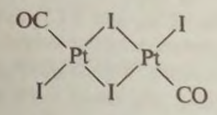
M 753.8 (ion)

trans-form
Tetrabutylammonium salt: [55399-54-7].
Deep-green platelets (CH_2Cl_2). Sol. Me_2CO, CH_2Cl_2, $CHCl_3$, DMF, mod. sol. EtOH.

Preetz, W. *et al, J. Organomet. Chem.*, 1975, **86**, 397 (*synth, ir, uv*)

IC-003442

$C_2I_4O_2Pt_2$
Dicarbonyldi-μ-iododiodiplatinum(*II*), 11CI
Dicarbonyltetraiododiplatinum
[106863-40-5]



M 953.7
Dark violet cryst. (toluene). Ir ν_{CO} 2104 cm^{-1} (toluene). Reacts with CO.

Calderazzo, F. *et al, Pure Appl. Chem.*, 1986, **58**, 561 (*synth, ir*)
Andreini, B.P. *et al, J. Organomet. Chem.*, 1988, **354**, 357 (*synth, struct, ir*)

IC-003443

$C_2I_4O_2Rh^{\ominus}$
Dicarbonyltetraiodorhodate(1−), 10CI
Tetraiododicarbonylrhodate(1−)

$[RhI_4(CO)_2]^{\ominus}$

M 666.5 (ion)
Catalyst for the water-gas shift reaction and for hydrogenolysis of MeOH.

cis-form
Isom. to the *trans*-form within a few minutes at r.t.
Et_4N salt: [24596-69-8].

Characterised spectroscopically. Ir ν_{CO} 2122, 2092 cm^{-1} ($CHCl_3$).

trans-form [44769-93-9]
Tetrapropylammonium salt: [55634-00-9].
Black cryst. (CH_2Cl_2/CCl_4). Ir ν_{CO} 2091 cm^{-1} (CH_2Cl_2).
Tetrabutylammonium salt: [55634-01-0].
Black cryst.
Ph_4As salt: [26004-02-4].
Black cryst.

Forster, D., *Inorg. Chem.*, 1969, **8**, 2556 (*synth, ir*)
Daly, J.J. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2551 (*synth, struct*)
Drury, D. *et al, J. Organomet. Chem.*, 1982, **236**, C23 (*use*)

$C_2I_4O_3Ru^{2\ominus}$
Dicarbonyltetraiodoruthenate(2−), 8CI **IC-003444**
$[Ru(CO)_2I_4]^{2\ominus}$

M 664.7 (ion)

cis-form
Di-Cs salt: [16369-44-1].
Orange cryst.

Cleare, M.J. *et al, J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Colton, R. *et al, Aust. J. Chem.*, 1971, **24**, 903 (*ir*)

$C_2I_4O_4Os^{2\ominus}$
Tetraiodo(oxalato)osmate(*IV*)(2−) **IC-003445**
[*Ethanedioato*(2−)-O,O']*tetraiodoosmate*(IV)(2−), *10CI*
[74325-56-7]
As Tetrabromo(oxalato)osmate(*IV*)(2−), IC-002845 with

X = I

M 785.8 (ion)
Synth. from oxalic acid and $K_2[OsI_6]$.
Di-Cs salt: [74325-50-1].
Blue-green.
Bis-(Bu_4N) salt: [74325-57-8].
Ir ν_{Os-I} 178 cm^{-1}.

Homborg, H. *et al, Z. Naturforsch., B*, 1980, **35**, 554 (*synth, ir, uv, raman*)
Preetz, W. *et al, Z. Naturforsch., B*, 1981, **36**, 62 (*synth, ir, uv*)

$C_2InN_2O_2^{\ominus}$
Bis(cyanato-*O*)indate(1−) **IC-003446**
Di(cyanato)indate(1−)

$[In(OCN)_2]^{\ominus}$

M 198.8 (ion)
Synth. from $[Et_4N][InCl_2]$ and Na[NCO]. Not clear whether ligand bound through O or N.
Et_4N salt: [60131-20-6].
Colourless moisture-sensitive cryst. (EtOH).

Habeeb, J.J. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 866 (*synth, ir*)

$C_2InN_2S_2^{\ominus}$
Bis(thiocyanato-*S*)indate(1−) **IC-003447**

$[In(SCN)_2]^{\ominus}$

M 230.9 (ion)
Synth. from $[Et_4N][InCl_2]$ and Na[NCS]. Not clear whether ligand bound through N or S.
Et_4N salt: [60131-18-2].

Colourless moisture-sensitive cryst. (EtOH).

Habeeb, J.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 866 (*synth, ir*)

IC-003448

$C_2K_2O_4$

Potassium oxalate

Oxalic acid, dipotassium salt, 8CI. Ethanedioic acid, dipotassium salt, 9CI

[583-52-8]

$K_2(C_2O_4)$

M 166.2

Synth. by reaction of KOH with aq. oxalic acid, cryst. as monohydrate which dehydrates at ~ 100°. Hygroscopic colourless orthorhombic cryst. Becomes tetragonal at 381°. Dec. above 470° to CO and K_2CO_3. ΔH_f° −1342 kJ mol^{-1}.

▷ RO2885000.

Monohydrate: [6487-48-5].
$C_2H_2K_2O_5$ M 184.2
Commercially available. Cryst. from aq. solns. of $K_2C_2O_4$. White monoclinic cryst.; hygroscopic. Dec. on heating with H_2O loss (− H_2O at ~ 100°). V. sol. H_2O (33 g per 100 cm^3 at 16°). ΔH_f° −1641 kJ mol^{-1}.

▷ Irritant.

Graddon, D.P., *Chem. Ind. (London)*, 1956, 80 (*uv*)
Collman, J.P. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 2054 (*ir*)
Pedersen, B.F., *Acta Chem. Scand.*, 1964, **18**, 1635 (*struct, monohydrate*)
Bardet, L. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1967, **265**, 983 (*ir, raman*)
Sequira, A. *et al*, *Acta Crystallogr., Sect. B*, 1970, **26**, 77 (*monohydrate, struct*)
Hiyashiyama, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 1727 (*polymorphs, struct*)
Verdonk, A.H., *Therm. Anal., Proc. Int. Conf., 3rd, 1971*, 1971, **2**, 651, *CA*, 1973, **78**, 131588 (*thermal dec, monohydrate*)
Fabbri, G. *et al*, *CA*, 1977, **86**, 182308 (*thermal dec*)
Eriksson, A. *et al*, *Acta Chem. Scand., Ser. A*, 1978, **32**, 737 (*ir, monohydrate*)
Ebisuzaki, Y. *et al*, *J. Raman Spectrosc.*, 1981, **11**, 306 (*raman, monohydrate*)
Ratcliffe, C.I. *et al*, *Chem. Phys. Lett.*, 1985, **120**, 427 (*pmr, monohydrate*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2907A (*haz*)

IC-003449

C_2Li_2

Dilithioethyne

μ-1,2-Ethynediyldilithium, 10CI. Lithium acetylide ($Li_2(C_2)$), 10CI, 8CI. Dilithium acetylide. Lithium carbide (Li_2C_2). Acetylene, dilithium salt. Ethyne, dilithium salt

[1070-75-3]

LiC≡CLi

M 37.9

Isotypic with Rb_2O_2. Prepd. by reaction of Li vapour with graphite at 800-900°. Acetylene source. Moisture-sensitive white cryst. V. thermodynamically stable. Reacts with H_2O to form LiOH and C_2H_2. Insol. org. solvs. ΔH_f° −59 kJ mol^{-1}; ΔG_f° −66 kJ mol^{-1}.

Inhoffen, H.H. *et al*, *Justus Liebigs Ann. Chem.*, 1949, **565**, 45 (*synth, use*)
Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 494 (*rev, bibl*)
Juza, R. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **352**, 252 (*cryst struct, synth*)
Shimp, L.A. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 5951.

Ritchie, J.P., *Tetrahedron Lett.*, 1982, **23**, 4999 (*struct*)
Chase, M.W. *et al*, *J. Phys. Chem. Ref. Data, Suppl. 1*, 1985, **14**, 664 (*thermochem, data*)

IC-003450

$C_2Li_2O_4$

Lithium oxalate

Dilithium ethanedioate, 9CI. Oxalic acid, dilithium salt, 8CI. Ethanedioic acid, dilithium salt

[553-91-3]

Li(OOCCOO)Li

M 101.9

Prepd. by neutralisation of LiOH with oxalic acid in aq. soln. Colourless monoclinic cryst. Dec. on heating. Mod. sol. H_2O (8g per 100 cm^3 at 20°); insol. EtOH, Et_2O. ΔH_f° −1376.6 kJ mol^{-1}.

Gmelin Handbook Inorg. Chem., Syst. No. 20, 1960, 510 (*rev, bibl*)
Beagly, B., *Acta Crystallogr.*, 1964, **17**, 783 (*cryst struct*)
Pederson, B.F., *Acta Chem. Scand.*, 1967, **21**, 801 (*ir*)
Kazin, I.V., *Zh. Fiz. Khim.*, 1984, **58**, 37 (*thermodynamics*)

IC-003451

C_2MnN_2

Manganese(*II*) cyanide ($Mn(CN)_2$)

$Mn(CN)_2$

M 106.9

Mentioned in the older literature but the pure compd. has not been isol. Some adducts with NH_3, DMSO, DMF have been described. Treatment of $K_3Mn(NO)(CN)_5$ with H_2 at 330° gives a dark brown solid of empirical formula $Mn(CN)_{2.1}$. μ_{eff} = *ca.* 4.23μ_B; Ir ν_{CN} 2140 cm^{-1}.

DMSO complex: see *Dicyano(dimethyl sulfoxide) manganese*(II), *IC-004019*

DMF complex: [71072-53-2].
Synth. from $MnCl_2$ and $[NH_4]CN$ in DMF.

Diammine complex: Obt. from corresp. hexaammine complex. Oxygen and moisture sensitive pale yellow green solid. Magnetic data indicate formulation $[Mn(NH_3)_4][Mn(CN)_4]$? with high spin cation and low spin cation. Hydrol. with H_2O gives dark green solid of composition $Mn(CN)_2$.

Hexaammine complex:
$C_2H_{18}MnN_8$ M 209.1
Synth. from $Mn(NCS)_2$ and KCN in liq. NH_3 at −40°. Oxygen and moisture sensitive bright pink solid. Loses NH_3 *in vacuo* to form $Mn(CN)_2(NH_3)_2$.

Nast, R. *et al*, *Z. Anorg. Allg. Chem.*, 1957, **293**, 322 (*synth, hexaammine complex*)
Banks, D.F. *et al*, *Inorg. Chem.*, 1967, **6**, 1849 (*synth, props, $Mn(CN)_{2.1}$*)
Kuntyi, O.I. *et al*, *Koord. Khim.*, 1979, **5**, 685 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, **C7**, 229; 1982, **D3**, 18 (*rev, bibl*)

IC-003452

$C_2MnN_2O_4^{\ominus}$

Dicarbonyldinitrosylmanganate(1−)

$[Mn(CO)_2(NO)_2]^{\ominus}$

M 170.9 (ion)

Bis(triphenylphosphine)iminium salt: [79061-79-3].
Synth. from $[Mn(CO)_6]BF_4$ and $[Ph_3PNPPh_3]NO_2$ in MeCN. Orange.

Stevens, R.E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4981.
Stevens, R.E. *et al*, *Inorg. Chem.*, 1983, **22**, 2034 (*cryst struct*)

IC-003453

$C_2MnN_2S_2$

Manganese(*II*) thiocyanate

Bis(thiocyanato) manganese, 8CI. Dithiocyanatomanganese

[25853-88-7]

$Mn(SCN)_2$

M 171.1

Ir spectra suggest tetragonal coordination with SCN bridges. Synth. from $MnCl_2$ or $Mn(NO_3)_2$ and KSCN in EtOH followed by drying *in vacuo* at 110° over P_2O_5. Sol. H_2O, EtOH, liq. NH_3. Reacts with Br_2 (g) to give Mn(SCN)Br. $Mn(SCN)_2.3H_2O$ is described in the older literature.

Sundheim, B.R., *Anal. Chem.*, 1958, **30**, 1892 (*esr*)
Flint, C.D. *et al*, *J. Chem. Soc. A*, 1970, 442 (*synth, ir, uv, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1981, C7, 234 (*rev, bibl*)

IC-003454

$C_2MnN_4O_2^{3\ominus}$

Bis(cyano-*C*)dinitrosylmanganate(3−)

Dicyanodinitrosylmanganate(-I)

$[(ON)_2Mn(CN)_2]^{3\ominus}$ (C_{2v})

M 166.9 (ion)

▷ Pyrophoric.

Tri-K salt: [26470-94-0].
$C_2K_3MnN_4O_2$ M 284.2
Synth. from $K_4[Mn_2(CN)_4(NO)_4]$ and K in liq. NH_3. Air-sensitive greenish solid. Ir ν_{CN} 2038s, 2017vs; ν_{NO} 1455s, 1425vs cm^{-1} (KBr). Diamagnetic.

Behrens, H. *et al*, *Z. Anorg. Allg. Chem.*, 1969, **365**, 119 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 279 (*rev, bibl*)
Compr. Organomet. Chem., Pergamon, Oxford, 1982, **4**, 1 (*rev, bibl*)

IC-003455

C_2MnO_4

Manganese(*II*) oxalate

[Ethanedioato(2−)-O,O′]manganese, 11CI

[640-67-5]

$Mn(O_2CCO_2)$

M 142.9

Pink cryst. Synth. by heating dihydrate in N_2 for 2hr at 200°. ΔH_{298}° −1087.3 kJ mol^{-1}.

Manganese(II) oxalate dihydrate [6556-16-7]
Diaqua[ethanedioato(2−)-O,O′]manganese, 11CI
$C_2H_4MnO_6$ M 178.9
Possesses polymeric chain struct. with *trans*-octahedral Mn and bridging oxalate groups. ΔH°_{298} −1624.5 kJ mol^{-1}.

α-form: Formed from damp trihydrate at r.t., or from aq. solns. of $Mn^{2\oplus}$ and $C_2O_4^{2\ominus}$ above 30° at pH 1.5. Monoclinic colourless cryst.

γ-form: Formed from aq. solns. of $Mn^{2\oplus}$ and $C_2O_4^{2\ominus}$ above 30° at pH 3-6. Orthorhombic pink cryst. More thermally stable than α-form.

Manganese(II) oxalate trihydrate [74174-53-1]
[Ethanedioato(2−)-O,O′]manganese trihydrate
$C_2H_6MnO_7$ M 213.0
Synth. by mixing aq. solns. of $Mn^{2\oplus}$ and $C_2O_4^{2\ominus}$ below 30° at pH 1.5-6. Orthorhombic pink prisms.

[55703-32-7, 88682-90-0]

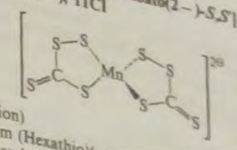
Dollimore, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1969, 2946 (*synth, thermal dec, struct*)

Deyrieux, R. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 25 (*cryst struct*)
Nagase, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 439 (*thermal dec, ir*)
Deyrieux, R. *et al*, *J. Chem. Phys.*, 1975, **72**, 793 (*thermodyn props*)
Huizing, A. *et al*, *Mater. Res. Bull.*, 1977, **12**, 605 (*synth, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, D2, 89 (*rev, bibl*)

IC-003456

$C_2MnS_8^{2\ominus}$

Bis[carbono(dithioperoxo)dithioato(2−)-*S,S′*] manganate(*II*)(2−), 11CI



M 335.4 (ion)

Synth. from (Hexathio)(pentathio)manganate(*II*)(2−), IC-020738 and CS_2 in DMF.

Bis-Ph_4P salt: [93714-72-8].
Orange-red cryst. + 1DMF; unstable in air.

Coucouvanis, D. *et al*, *Inorg. Chem.*, 1985, **24**, 24 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, D7, 210 (*rev, bibl*)

IC-003457

C_2N_2

Cyanogen

Ethanedinitrile, 9CI. Oxalonitrile. Dicyanogen

[460-19-5]

N≡C—C≡N ($D_{\infty h}$)

M 52.0

Interatomic distances: C—C 137 pm, C—N 116 pm.
Synth. from NaCN and $CuSO_4$. Colourless gas. Hydrol. first to oxamide, then to oxalic acid. Sol. H_2O, EtOH, Et_2O. d_4^{21} 0.954. Mp −27.9°. Bp −21.17°. Burns with violet flame → CO_2 + N_2. V.p., 2.4 atm. at 0°. Heating above 400° → Paracyanogen, a polymer which reverts to cyanogen. at 500°.

▷ Toxic vapour, irritant. Extremely flammable. GT1925000.

Walden, P. *et al*, *Chem. Rev.*, 1928, **5**, 339
Inorg. Synth., 1957, **5**, 43 (*synth*)
Maki, A.G., *J. Chem. Phys.*, 1965, **43**, 3193 (*struct*)
Weigert, W. *et al*, *Ullmanns Encykl. Tech. Chem.*, 4. Aufl., 1975, **9**, 655 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 628 (*synth*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 407.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 986.

IC-003458

C_2N_2

Cyanoisocyanogen

[83951-85-3]

CN—CN

M 52.0

Originally descr. as Diisocyanogen, CN—NC. Formed by flash photolysis of norbornadienone azine at 500°. Dec. > −30° with formation of brown polymer.

[78800-21-2]

van der Does, T. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1988, **27**, 936 (*synth, ms*)

Cederbaum, L.S. *et al, Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 761 (*pe, struct*)
Stroh, F. *et al, Chem. Phys. Lett.*, 1989, **155**, 21 (*comb, ir, microwave*)

IC-003459

C_2N_2Ni

Nickel(*II*) cyanide ($Ni(CN)_2$)

[557-19-7]

$Ni(CN)_2$

M 110.7
Struct. not known. *Synth.* from Hexaaquanickel(*II*)(2+), IC-015897 + $CN^{\ominus}$ (not excess), followed by heating to 180-200°. Grey-brown or yellow-brown solid (reports conflict). Sol. MeOAc.

▷ QR6495000.

Inorg. Synth., 1946, **2**, 228 (*synth*)
Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1434.
Remy, H., *Treatise on Inorg. Chem.*, Elsevier, 1956, **2**, 315.
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1698 (*synth*)

IC-003460

$C_2N_2NiS_2$

Nickel(*II*) thiocyanate

Bis(thiocyanato)nickel, 8CI

[13689-92-4]

$Ni(NCS)_2$

M 174.8
Synth. from $NiCO_3$ + HNCS, $Ba(NCS)_2$ + $NiSO_4$ (aq.) or $Ni^{2\oplus}$ and $(NH_4)SCN$ in aq. AcOH. Brown solid. Sol. H_2O. Ir $\nu_{C\equiv N}$ 2151 cm^{-1}.

Hemihydrate: [97128-57-9].
Yellow solid. Sol. H_2O. Obtd. on cryst. of soln. >15°.

Tetrahydrate:
$C_2H_8N_2NiO_4S_2$ M 246.9
Obtd. by metathesis from $NiSO_4$ and $Ba(NCS)_2$. Green cryst. (obt. <15°). Sol. H_2O.

Mitchell, P.C.H. *et al, J. Chem. Soc.*, 1960, 1912 (*ir*)
Tramer, A., *J. Chem. Phys.*, 1962, **59**, 232 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1966, **B3**, 911 (*rev*)
Peters, W., *Chem. Ber.*, 1968, **41**, 3175 (*synth*)
Ali, S. *et al, Pol. J. Chem. (Rocz. Chem.)*, 1984, **58**, 659; 1985, **59**, 535 (*ir*)
Sarmi, K.P. *et al, Transition Met. Chem.*, 1984, **9**, 135 (*synth, deriv*)

IC-003461

C_2N_2O

Cyanoisocyanate

[22430-66-6]

$N{\equiv}CN{=}C{=}O$

M 68.0
Formed on thermal depolym. of $(C_2N_2O)_x$. White polymeric solid at −60°. At 20° and low press. gives the monomer.

Polymer: Synth. from AgCNO + ClCN at r.t. Yellow solid; v. sensitive to hydrol. Involatile at r.t. Ir ν_{CN} 2275; ν_{CO} 1770 cm^{-1}.

Mayer, E. *et al, Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 444 (*synth*)
Mayer, E., *Monatsh. Chem.*, 1970, **101**, 834 (*ir, reactions*)

IC-003462

$C_2N_2OS_2Ti$

Oxobis(thiocyanato-*N*)titanium(*IV*), 11CI

Dithiothiocyanatooxotitanium(IV). *Titanyl thiocyanate*

[104065-39-6]

$TiO(NCS)_2$

M 180.0
Synth. by thermal dec. of $TiO(S_2CNHR)_2$ (R = cyclopentyl or cycloheptyl).

Srivastava, A.K. *et al, Croat. Chim. Acta*, 1981, **54**, 329 (*deriv, ir*)
Pandey, O.P. *et al, J. Therm. Anal.*, 1986, **31**, 387 (*synth, ir*)

IC-003463

$C_2N_2OS_2Zr$

Oxobis(thiocyanato-*S*)zirconium(*IV*), 11CI

[72017-87-9]

$ZrO(SCN)_2$

M 223.3
Synth. from KNCS and $ZrO(NO_3)_2$ in MeOH. This compound is also formed in the dec. of $ZrO(S_2CNHR)_2$ (R = cyclopentyl).

Dihydrate:
$C_2H_4N_2O_3S_2Zr$ M 259.4
Synth. from $Zr(SO_4)_2$ and $Ba(NCS)_2$ in H_2O.

Tananaev, I.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 957 (*synth, dihydrate*)
Chopra, J.R. *et al, Croat. Chim. Acta*, 1982, **55**, 283 (*synth*)
Pandey, O.P. *et al, J. Therm. Anal.*, 1986, **31**, 387 (*synth*)

IC-003464

$C_2N_2OSe_2Zr$

Oxobis(selenocyanato-*N*)zirconium(*IV*)

$ZrO(NCSe)_2$

M 317.1
Isol. as various complexes by reaction of freshly prepared samples with a ligand. Synth. from $ZrO(NO_3)_2$ and KNCSe in MeOH.

Bis-hydrazine complex: [84291-86-1]. *Bis(hydrazine-N) oxobis(selenocyanato-N)zirconium*(IV), *11CI*
$C_2H_8N_6OSe_2Zr$ M 381.2

Bis-phenylhydrazine complex: [84291-87-2]. *Oxobis(phenylhydrazine-N^2)bis(selenocyanato-N) zirconium*(IV), *11CI*
$C_{14}H_{16}N_6OSe_2Zr$ M 533.4
Colourless, air-stable solid. Insol. MeOH, Et_2O.

Bis-Py complex: [84291-82-7]. *Oxobis(pyridine) bis(selenocyanato-N)zirconium*(IV), *11CI*
$C_{12}H_{10}N_4OSe_2Zr$ M 475.3
Colourless air-stable solid. Insol. MeOH, Et_2O.

Bis(2,4-dimethylpyridine) complex: [84291-83-8]. *Bis(2,4-lutidine)oxobis(selenocyanato-N)zirconium*(IV)
$C_{16}H_{18}N_4OSe_2Zr$ M 531.4

Phen complex: [84291-85-0]. *Oxobis(1,10-phenanthroline-N^1,N^{10})bis(selenocyanato-N)zirconium*
Colourless moisture-sensitive solid. Insol. MeOH, Et_2O.

Chopra, J.R. *et al, Croat. Chim. Acta*, 1982, **55**, 283 (*deriv, synth, ir*)

IC-003465

$C_2N_2O_2Pb$

Lead(*II*) cyanate

[13453-58-2]

$Pb(OCN)_2$

M 291.2

White needles. Insol. cold H_2O; sl. sol. hot H_2O. Dec. on heating.

Rao, C.N.R. *et al, J. Sci. Ind. Res., Sect. B*, 1959, **18**, 169 (*ir*)
U.S. Pat., 3 116 107, (1963); *CA*, **60**, 8931 (*synth*)
Becker, B. *et al, Z. Anorg. Allg. Chem.*, 1976, **422**, 89
Nefedov, V.I. *et al, Zh. Neorg. Khim.*, 1979, **24**, 2564 (*pe*)

IC-003466

$C_2N_2O_2S_2U$

Dioxobis(thiocyanato-*S*)uranium(*VI*)

Uranyl thiocyanate

[21696-47-9]

$UO_2(SCN)_2$

M 386.1
Usually obt. as trihydrate. V. dark green solid. Virt. insol. H_2O. Reacts with range of donor ligands, forming adducts.

Trihydrate: [83650-98-0].
Orange powder. Sol. H_2O. Ir $\nu_{C\equiv N}$ 937 cm^{-1}; $\nu_{C=N}$ 2057 cm^{-1}. Loses H_2O of cryst. at 85-125°.

Pascal, R., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1914, **158**, 1672 (*synth*)
Markov, V.P. *et al, Zh. Neorg. Khim.*, 1960, **5**, 1467; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1960, **5**, 712 (*synth*)
Shchelokov, R.N. *et al, Zh. Neorg. Khim.*, 1967, **12**, 1246; 1982, **27**, 2348; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 660; 1982, **27**, 1314 (*synth, reactions*)
Vdovenko, V.M. *et al, Zh. Neorg. Khim.*, 1968, **13**, 3059; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1577 (*reactions, ir*)

IC-003467

$C_2N_2O_4Os$

Dicarbonyldinitrosylosmium, 9CI

[42718-59-2]

$Os(CO)_2(NO)_2$

M 306.2
Characterised spectroscopically.

Crichton, O. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1321.

IC-003468

$C_2N_2O_4S$

Sulfuryl isocyanate

[4223-09-0]

$O_2S(NCO)_2$

M 148.0
Formed from BrCN + SO_3. Colourless liq., violently hydrol. Bp 135°.

Ger. Pat., 940 351, (1956); *CA*, **52**, 12344d (*synth*)
Neffe, R. *et al, Inorg. Chem.*, 1968, **7**, 687 (*synth, reactions*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 492 (*synth*)

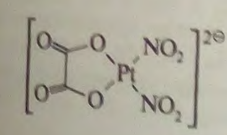
IC-003469

$C_2N_2O_8Pt^{2\ominus}$

Dinitrito(oxalato)platinate(*II*)(2−)

[Ethanedithioato(2−)-O,O']bis(nitrito-N)platinate(II)(2−), *9CI. Dinitro(oxalato)platinate*(II)(2−), *8CI*

[54516-14-2]



M 375.1 (ion)

IC-003470

C_2N_2Pb

Lead(*II*) cyanide

Lead dicyanide

[592-05-2]

$Pb(CN)_2$

M 259.2
Yellowish/white powder. Sl. sol. cold H_2O; sol. hot H_2O, sol. aq. KCN.

▷ Poisson. OG0175000.

Rao, C.N.R. *et al, J. Sci. Ind. Res., Sect. B*, 1959, **18**, 169 (*ir*)
Wilcox, D.E. *et al, Ind. Eng. Chem.*, 1963, **55**, 32.
Kroeker, R.M. *et al, J. Chem. Phys.*, 1982, **77**, 4935.

IC-003471

$C_2N_2PbS_2$

Lead(*II*) thiocyanate

Thiocyanic acid, lead(2+) salt, 9CI

[592-87-0]

$Pb(SCN)_2$

M 323.3
Synth. by mixing aq. solns. of NaSCN and $Pb(NO_3)_2$. White needles. Light sensitive. Insol. H_2O. Mp 190° dec.

▷ Toxic. XL1538000.

Inorg. Synth., 1939, **1**, 55 (*synth*)
Mokuolu, J.A.A. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 172 (*cryst struct*)

IC-003472

C_2N_2Pd

Palladium(*II*) cyanide ($Pd(CN)_2$), 8CI

[2035-66-7]

$Pd(CN)_2$

M 158.4
Probably polymeric struct. Few modern studies. *Synth.* from $Pd^{2\oplus}$(aq.) + $Hg(CN)_2$. Yellow solid.

[69860-44-2]

Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1561.

IC-003473

$C_2N_2Pt^{2\ominus}$

Dicyanoplatinate(2−), 8CI

$[Pt(CN)_2]^{2\ominus}$

M 247.1 (ion)
Probably has polymeric struct. *Synth.* from Tetrakis(cyano-*C*)platinate(2−), IC-004558 + K/NH_3.

Bis-Ph_4P salt: [22784-73-2].
Brick red solid.

Nast, R. *et al, Chem. Ber.*, 1969, **102**, 1050 (*synth*)

IC-003474

C_2N_2Pt

Platinum(*II*) cyanide ($Pt(CN)_2$)

[592-06-3]

$Pt(CN)_2$

M 247.1
Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + $Hg(CN)_2$. Reacts with KCN → Tetrakis(cyano-*C*)platinate(2−), IC-004558. Pale yellow solid. Insol. H_2O, acids, alkalis.

Gmelin Handbook Inorg. Chem., Syst. No. 68, 1940, C, 123 (*rev, bibl*)
Sidgwick, N.V., *The Chemical Elements and their Compds.*, Oxford, 1950, 1582.

IC-003475

C_2N_2S
Sulfur dicyanide
Sulfur cyanide ($S(CN)_2$). *Dicyano sulfide. Dicyanosulfane*

N≡C—S—C≡N (C_{2v})

M 84.1
Interatomic distances: N—C 115.7, C—S 170.1 pm. Formed from AgCN + SCl_2 in CS_2. Colourless cryst. solid, dec. in air. V. sol. Et_2O, CS_2. Mod. sol. H_2O. Mp 64°.

Long, D.A. *et al, Spectrochim. Acta*, 1963, **19**, 1731 (*synth, ir, raman*)
Pierce, L. *et al, J. Chem. Phys.*, 1965, **43**, 3423 (*struct*)
Moren, M. *et al, J. Organomet. Chem.*, 1979, **165**, 215 (*metal complexes*)

IC-003476

$C_2N_2S_2$
Thiocyanogen, 9CI, 8CI
Disulfidodicarbonitrile. Dicyanodisulfide. Dirhodan. Rhodan. Thiocyan
[505-14-6]

$(SCN)_2$

M 116.1
Synth. from $Pb(SCN)_2$ + Br in acetic acid/anhydride. White cryst. or orange liq. Stable as 0.1M soln. over 8d. Mp 15-16°. Rapidly hydrol. to HCN + HNCS + H_2SO_4.

▷ Explosive at 20°.

Inorg. Synth., 1939, **1**, 84 (*synth as soln*)
Nelson, M.J. *et al, J. Chem. Soc.*, 1960, 604 (*ir*)
Bacon, R.G.R., *Org. Sulfur Compd.*, 1961, **1**, 306 (*rev*)
Feher, F. *et al, Chem. Ber.*, 1963, **96**, 1131 (*synth, uv*)
Welcher, R.P. *et al, J. Org. Chem.*, 1972, **37**, 4478 (*synth, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 671 (*synth*)
Guy, R.G., *The Chemistry of Functional Groups, The Chemistry of Cyanides and their Thio Derivatives*, (ed. Patai, S.), Part 2, Wiley-Interscience, 1977, 819 (*rev*)
Jensen, N.H. *et al, J. Chem. Phys.*, 1979, **71**, 3326 (*ir*)
Frost, D.C. *et al, Chem. Phys. Lett.*, 1980, **69**, 1 (*synth, bibl, struct, uv, pe*)

IC-003477

$C_2N_2S_2Se$
Dithiocyanatoselenium
Selenium thiocyanate ($Se(SCN)_2$)
[60763-20-4]

N≡CSSeSC≡N

M 195.1
Synth. from NH_4SCN + SeO_2 + HCl. Cryst. solid stable in dark at low temps. Dec. to Se + $S_2(CN)_2$. Hydrol. by H_2O. Sol. H_2O, dioxan. Mp 83° dec.

Ohlberg, S.M. *et al, J. Am. Chem. Soc.*, 1953, **75**, 997; 1954, **76**, 2649 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1978, **D6**, 256, 263 (*bibl*)

$C_2N_2S_2Sn$
IC-003478
Tin(*II*) thiocyanate
Thiocyanic acid, tin(2+) salt, 9CI. Stannous thiocyanate
[3602-20-8]

$Sn(SCN)_2$

M 234.8
Sn atoms surrounded by 9 SCN groups - not all in primary coordination, Sn considered to have distorted tetrahedral or octahedral coordination (*cf* $PbCl_2$). Synth. from $SnSO_4$ + NaNCS. Cryst. Dec. >150°. Spar. sol. H_2O, Et_2O, EtOAc; sol. MeOH, EtOH.

Chamberlain, B.R. *et al, J. Chem. Soc. A*, 1969, 354 (*synth*)
Absi, T.B. *et al, Can. J. Chem.*, 1978, **56**, 2039 (*ir, raman*)
Herber, R.H. *et al, Inorg. Chem.*, 1978, **17**, 1023 (*mössbauer*)
Filby, A.G. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 1797 (*cryst struct*)
Abiedu, A.M. *et al, Indian Chem. J.*, 1979, **13**, 29 (*synth, ir*)

IC-003479

$C_2N_2S_2Zn$
Zinc thiocyanate
Thiocyanic acid, zinc salt. Bis(thiocyanato)zinc
[557-42-6]

$Zn(NCS)_2$

M 181.5
Zn—N bonded in soln. In solid state, NCS bridges Zn to give two T_d environments: ZnN_4 and ZnS_4. Cryst. Thermal dec. to ZnS.

Spacu, G. *et al, Z. Anorg. Allg. Chem.*, 1936, **227**, 129.
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 986 (*rev, bibl*)
Golub, A.M. *et al, Zh. Neorg. Khim.*, 1958, **3**, 333 (*synth*)
Flint, C.D. *et al, J. Chem. Soc. A*, 1970, 442 (*synth, ir*)
Aslanov, L.A. *et al, Kristallografiya*, 1976, **21**, 1198 (*cryst struct*)
Zurano Hernandez, G. *et al, An. Quim.*, 1977, **73**, 820 (*cryst struct*)
Persson, I. *et al, Acta Chem. Scand., Ser. A*, 1981, **35**, 295 (*raman*)

IC-003480

$C_2N_2S_3$
Trisulfur dicyanide
Dicyanotrisulfane. Dicyano trisulfide
[57670-85-6]

N≡CSSSC≡N

M 148.2
Synth. from S_2Cl_2 + AgCN in CS_2. White cryst. stable at −20°. Polym. on heating. Dec. by H_2O. Sol. Et_2O, $CHCl_3$, C_6H_6. Mp 93°.

Feher, F. *et al, Z. Anorg. Allg. Chem.*, 1964, **327**, 151 (*synth, cryst struct*)

IC-003481

$C_2N_2S_4$
Tetrasulfur dicyanide
Dicyanotetrasulfane. Dicyano tetrasulfide

N≡CSSSSC≡N

M 180.2
Formed from S_2Cl_2 + $Hg(SCN)_2$. Colourless cryst. Readily polym. to other cyanosulfanes. Dec. by H_2O. Sol. $CHCl_3$, CCl_4, CS_2. Mp −3.3°.

Feher, F. *et al, Chem. Ber.*, 1958, **91**, 642 (*synth, ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1977, **D5**, 235 (*bibl*)

C_2N_2Se
Selenium dicyanide IC-003482
Dicyano selenide. Selenium(II) *cyanide. Dicyanoselane*

N≡C—Se—C≡N (C_{2v})

M 130.9
Formed from $SeCN^{\ominus}$ + N_2O_4 or from BrCN + KSeCN. Colourless cryst.

Aynsley, E.E. *et al, J. Chem. Soc.*, 1964, 704 (*synth*)
Hange, S., *Acta Chem. Scand.*, 1971, **25**, 3081 (*synth, reactions*)
Moran, M. *et al, J. Organomet. Chem.*, 1979, **165**, 215 (*metal complexes*)

$C_2N_2Se_2$
Diselenium dicyanide IC-003483
Dicyanodiselane. Dicyano diselenide
[2180-01-0]

N≡CSeSeC≡N

M 209.9
Formed from 2AgSeCN + I_2 in Et_2O. Yellow cryst. Sol. org. solvs. Dec. at 20° to $Se(CN)_2$ + $Se_3(CN)_2$.

Birckenbach, L. *et al, Ber.*, 1925, **58**, 786 (*synth*)
Aynsley, E.E. *et al, J. Chem. Soc.*, 1964, 704 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1978, **D6**, 235 (*bibl*)

$C_2N_2Se_3$
Triselenium dicyanide IC-003484
Dicyanotriselenide, 9CI. Selenium diselenocyanate. Dicyanotriselane
[2179-96-6]

N≡CSeSeSeC≡N

M 288.9
Formed by thermal dec. of $Se_2(CN)_2$. Yellow cryst. (C_6H_6). Sol. org. solvs. Mp 132° dec., Mp 133° (150°). Dec. at 148°. Subl. *in vacuo*.

Muthmann, W. *et al, Ber.*, 1900, **33**, 1765 (*synth*)
Kaufmann, H.P. *et al, Ber.*, 1926, **59**, 178 (*synth*)
Rheinboldt, H. *et al, J. Am. Chem. Soc.*, 1949, **71**, 1740 (*synth*)
Asknes, O. *et al, Acta Chem. Scand.*, 1954, **8**, 1787 (*cryst struct*)
Aynsley, E.E. *et al, J. Chem. Soc.*, 1965, 2395 (*synth*)
Hange, S., *Acta Chem. Scand.*, 1971, **25**, 3081 (*synth, bibl*)

C_2N_2Sn
Tin(*II*) cyanide IC-003485
Bis(cyano-C)tin
[35667-77-7]

$Sn(CN)_2$

M 170.7
Prepd. by addition of HCN to a THF soln. of bis(methylcyclopentadienyl)tin. White solid. Air-sensitive.

Harrison, P.G. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 940 (*synth, mössbauer, ir*)

C_2N_2Te
IC-003488
Tellurium dicyanide
Dicyano telluride. Tellurium(II) *cyanide. Dicyanotellane*
[14453-24-8]

N≡C—Te—C≡N

M 179.6
Synth. from $TeBr_4$ + AgCN in C_6H_6. Orange solid. Sol. Et_2O. Subl. 120° in vacuo. Dec. at 80°.

Cockerage, H.E., *J. Chem. Soc.*, 1968, **90**, 2075 (*synth*)
Aranda, T. *et al, Acta Chem. Scand., Ser. A*, 1974, **28**, 891 (*synth, reactions*)

C_2N_2Vo
Bis(cyano-Cyanamidato(2−), 11Cl IC-003487
Dicyanoamidato(2−)

$[V(CN)_2]^{2\ominus}$

M 102.9 (ion)
No struct. reported.
Di-K salt, hemiammoniate: [82720-69-3]
Synth. by K reduction of VBr_3 + KCN in liq. NH_3. Dark brown solid. Paramagnetic, μ_{eff} = 1.86 μ_B, S = 1/2. 2.09Å. Oxidised to Tetrakis(cyano-Cyanamidato)*II*(2−), IC-004567 by $[NH_4]CN$.
▷ Cyanides are toxic.

Dodsworth, E.S. *et al, Inorg. Chim. Acta*, 1982, **61**, 9 (*synth, ir, magnetism, uv-vis*)

C_2N_2Zn
Zinc cyanide
[557-21-1]

IC-003489

$Zn(CN)_2$

M 117.4
Cu_2O struct. Colourless cryst. Insol. EtOH, sol. aq. alkali cyanide and aq. NH_3, spar. sol. H_2O (5 × 10^{-4} g in 100 cm^3 at 20°). Mp 800° dec.
▷ Reported to be tasteless but poisonous. ZH 1 575000.

Blitz, W., *Z. Anorg. Allg. Chem.*, 1928, **170**, 101.
Swanson, W.E. *et al, Natl. Bur. Stad. Circ. (U.S.)*, 1955, **5**, No. 537 (powder struct)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 964.
Kirk-Othmer Encycl. Chem. Technol., 2nd Ed., Wiley, N.Y., 1965-1971, **22**, 604.
Wyckoff, W.C., *Cryst. Struct., Interscience*, 1965, **3**, 88, 146.
Persson, H. *et al, Acta Chem. Scand.*, 1971, **25**, 543 (*stability constr*)
Dehmicke, G. *et al, Ber. Bunsenges. Phys. Chem.*, 1974, **78**, 1010 (*ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1036 (*synth*)

C_2N_2Na
Sodium dicyanamide IC-003490
Cyanocyanamide sodium salt, 9CI. Dicyanamide, sodium salt, 8CI
[1934-75-4]

$NaN(CN)_2$

M 89.0
Synth. from solid BrCN + aq. NaNHCN. Manuf. by reaction of $M(N(CN)_2)_2$ (M = Ca, Zn, Cu) with aq. solns. of NaOH, Na_2CO_3 or Na_3PO_4. Commercially available. Widely used reagent in org. chem. Colourless cryst. Relatively stable but dec. on prolonged heating to $NaCN$, $(CN)_2$ and N_2. V. sol. H_2O (27 g per 100 cm^3 at 30°). Mp >315°.
▷ Irritant.

U.S. Pat., 2 455 895, (1948); *C.A.*, 1949, **43**, 1535d (*manuf*)
Kuhn, M. *et al, Chem. Ber.*, 1961, **94**, 3010 (*ir, synth*)
Takimoto, M., *Nippon Kagaku Zasshi (Jpn. J. Chem.)*, 1964, **85**, 159; *C.A.*, 61, 2937h (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1388 (*rev, bibl*)

Eur. Pat., 125 092, (1985); *CA*, **103**, 104579 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3139C (*haz*)

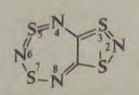
IC-003490

$C_2N_4S_4$

1,3,2-Dithiazolo[4,5-*e*][1,3,2,4,7]dithiatriazepine-3,5-S^{IV}, 9CI

$1\lambda^4\delta^2$,3,5,7$\lambda^4\delta^2$-Tetrathia-2,4,6,8-tetraazaazulene

[102298-87-3]



M 208.3
Planar 14π electron aromatic mol. Synth. from S_4N_4 + PhS(O)CH = CH_2. Green-black cryst. solid with metallic lustre, stable in hot C_6H_6. Mp 142-143°. Does not form charge-transfer complexes with electron acceptors.

Jones, R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 1654 (*synth, cryst struct, cmr*)

IC-003491

$C_2N_6O_{12}$

Hexanitroethane, 9CI, 8CI

[918-37-6]

$(O_2N)_3CC(NO_2)_3$

M 300.0
Formed by nitrating the K salt of trinitropropionaldehyde. High energy fuel oxidizer for rockets. Solid. Sol. CCl_4, CH_2Cl_2. Mp 150° dec.

▷ Highly toxic. KI4130000.

Wills, W., *Ber.*, 1914, **47**, 961 (*synth*)
Allsop, F. *et al*, *J. Chem. Soc.*, 1923, **123**, 2305 (*synth*)
Noble, P. *et al*, *CA*, 1963, **58**, 13701a (*props*)
U.S. Pat., 3 101 379, (1963); *CA*, **60**, 1588c (*synth*)
Laewenschluss, A. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 371 (*synth, ir, raman, ms*)

IC-003492

$C_2Na_2O_4$

Sodium oxalate

Sodium ethanedioate. Ethanedioic acid, disodium salt, 9CI. Oxalic acid, disodium salt, 8CI

[62-76-0]

$NaOOCCOONa$

M 133.9
Synth. by reaction of NaCl, with aq. oxalic acid. Manuf. either by thermal dec. of sodium formate or by treatment of sodium amalgam with CO_2. Commercially available. Constit. of aq. solns. used to anodise aluminium and its alloys and magnesium and its alloys. Colourless monoclinic cryst. Dec. on heating with evolution of CO and formation of Na_2CO_3. Mod. sol. H_2O (3.7 g per 100 cm^3 at 20°; 6.3g per 100 cm^3 at 100°); insol. EtOH, Et_2O. ΔH_f° −1315 kJ mol^{-1}.

▷ Irritant, toxic. KI1750000.

Shipman, J.J. *et al*, *Spectrochim. Acta*, 1962, **18**, 1603 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1440 (*rev, bibl*)
Kartha, V.B. *et al*, *Indian J. Phys., B*, 1980, **54**, 36; *CA*, 1981, **95**, 123260 (*raman*)
Reed, D.A. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 938 (*cryst struct*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3149A (*haz*)

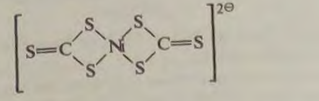
IC-003493

$C_2NiS_6^{2\ominus}$

Bis(trithiocarbonato)nickelate(*II*)(2−), 8CI

Bis(carbonotrithioato-S,S′)nickelate(II)(2−), *9CI*

[38840-58-3]



M 275.1 (ion)
Square planar struct.

Di-K salt: [21349-76-8].
$C_2K_2NiS_6$ M 353.3
Red-brown solid.

Bis-Ph_4As salt: [15083-84-8].
$C_{50}H_{40}As_2NiS_6$ M 1041.7
Red solid. Sol. MeCN, $MeNO_2$.

Hexaamminenickel(2+) salt: [51435-84-8].
$C_2H_{18}N_6Ni_2S_6$ M 435.9
Ruby-red solid. Previously formulated as $Ni(NH_3)_3CS_3$.

[38900-71-9]

Fackler, J.P. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 3913.
McKechnie, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 152 (*cryst struct*)
Burke, J.M. *et al*, *Inorg. Chem.*, 1972, **11**, 2744.
Müller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **401**, 274.
Stern, M. *et al*, *Rev. Chim. Minér.*, 1977, **14**, 40.

IC-003494

C_2O_2

Dicarbon dioxide

Carbon oxide (C_2O_2). *Ethenedione, 9CI*

[4363-38-6]

$OC{=}CO$

M 56.0
Not known. Calcns. suggest extreme instability.
Bis(dimethyl acetal): see *Tetramethoxyethene*, *IC-005162*
Bis(diethyl acetal): see *Tetraethoxyethene*, *IC-007101*
Hoffman, R.W. *et al*, *Tetrahedron*, 1965, **21**, 891.
Herberhold, M. *et al*, *Z. Naturforsch., B*, 1976, **31**, 35.

IC-003495

C_2O_4Pb

Lead(*II*) oxalate

Oxalatolead(II). *Lead*(II) *ethanedioate*

[814-93-7]

$Pb(C_2O_4)$

M 295.2
White powder. Spar. sol. H_2O, AcOH; sol. HNO_3; insol. EtOH. Dec. at 300°.

▷ Poisonous.

Yankwich, P.E. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 2081.
Robert, D., *Bull. Soc. Chim. Fr.*, 1960, 719.
Dollimore, D. *et al*, *J. Chem. Soc.*, 1963, 2617.
Debye, N.W.G. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 352 (*ir*)
Garten, V.A. *et al*, *J. Chem. Soc., Faraday Trans. 1*, 1973, **69**, 514.
Nejedov, V.I. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2564 (*pe*)

IC-003496

C_2O_4Sn

Tin(*II*) oxalate

Oxalatotin. Ethanedioic acid, tin(2+) salt (1:1). Stannous oxalate

[814-94-8]

$Sn(C_2O_4)$

M 206.7
Struct. has infinite chains in which Sn atoms and oxalate groups alternate. Synth. from $SnCl_2$ + oxalic acid. Esterification and hydrogenation catalyst. Insol. H_2O. Mp 280° dec.

▷ XQ3950000.

Gleizes, A. *et al*, *J. Solid State Chem.*, 1979, **30**, 23 (*cryst struct*)
Christie, A.D. *et al*, *Inorg. Chim. Acta*, 1979, **36**, L447 (*cryst struct*)
Debye, N.W.G. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 352 (*ir, mössbauer*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **23**, 69 (*use*)

IC-003497

C_2O_4Zn

Zinc oxalate

Ethanedioic acid, zinc salt (1:1), 9CI

[547-68-2]

$Zn(C_2O_4)$

M 153.4
White powder. Dimorphic.

Dihydrate: [4255-07-6].
$C_2H_4O_6Zn$ M 189.4
Prepd. from Zn salts + $(NH_4)_2C_2O_4$. Cryst. Prac. insol. H_2O. Dec. on heating above 100°, forming eventually ZnO.

Chatterjee, K.P. *et al*, *J. Phys. Chem.*, 1924, **28**, 1020 (*synth*)
Robin, J., *Bull. Soc. Chim. Fr.*, 1953, 1078 (*synth*)
Deyrieux, R. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 25 (*cryst struct, dihydrate*)
Nikonenko, E.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 547 (*ir, uv*)
Bogdonov, V.S. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1736 (*polymorphs*)
Kondrashev, Yu.D. *et al*, *Zh. Strukt. Khim.*, 1985, **26**, 90; *CA*, **102**, 195603d (*cryst struct*)

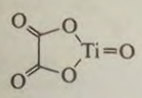
IC-003498

C_2O_5Ti

(Oxalato)oxotitanium(*IV*)

[*Ethanedioato*(2−)-O,O′]*oxotitanium*(IV), *11CI*

[31363-92-5]



M 151.8
Catalyst for polyester manuf.

Dihydrate: [80528-91-2].
Commercially available. White solid (H_2O). Forms Ti(*III*) on thermal dec.

Hydrate: [25592-02-3].
Synth. by precipitating titanium from $TiCl_4$ and dissolving the precipitate in saturated aq. oxalic acid. White solid.

Broadbent, D. *et al*, *Analyst* (*London*), 1969, **94**, 543 (*thermal anal, dihydrate*)
Japan. Pat., 70 27 110, (1970); *CA*, **74**, 4030k (*use*)
Japan. Pat., 78 101 093, (1978); *CA*, **89**, 216065k (*use*)
Nair, K.G. *et al*, *Thermochim. Acta*, 1980, **39**, 253 (*synth, thermal anal, hydrate*)
Gabelica-Robert, M. *et al*, *Proc. Eur. Symp. Therm. Anal.*, 2nd, 1981, 359; *CA*, **96**, 62153t (*thermal anal, esr, dihydrate*)

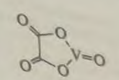
IC-003499

C_2O_5V

(Oxalato)oxovanadium(*IV*)

[*Ethanedioato*(2−)-O,O′]*oxovanadium*(IV), *11CI. Vanadyl oxalate*

[15500-04-6]



M 154.9
Synth. from V_2O_5 and $H_2C_2O_4$ in H_2O, or from V_2O_5 and $H_2C_2O_4$ in AcOH. Used in various catalytic processes including hydrocracking and EtOH to butadiene conversion. Also used to make V- containing metallurgical pellets. Blue solid.

Monohydrate: [39237-68-8].
Synth. from V_2O_5 and $H_2C_2O_4$.$2H_2O$ in AcOH at 108-118°.

Dihydrate: [39237-67-7].
Synth. analogously to monohydrate. A tetrahydrate is also known.

U.S. Pat., 3 689 515, (1972); *CA*, **78**, 15533k (*synth, anhyd form, hydrates*)
Netherlands Pat., 74 11 144, (1976); *CA*, **85**, 149641x (*use*)
Udupa, M.R., *Thermochim. Acta*, 1981, **51**, 169 (*thermal dec, dihydrate*)
Japan. Pat., 58 59 928, (1983); *CA*, **99**, 54864e (*use*)
Sasaki, Y. *et al*, *Sekiyu Gakkaishi*, 1983, **26**, 472; *CA*, **100**, 88291n (*synth, use*)

IC-003500

C_2O_5Zr

(Oxalato)oxozirconium(*IV*), 8CI

[*Ethanedioato*(2−)-O,O′]*oxozirconium*, *11CI. Zirconyl oxalate*

[25124-86-1]

$ZrO(C_2O_4)$

M 195.2
Synth. by adding $(NH_4)_2$ oxalate to aq. $ZrOCl_2$. Dec. on treatment with $Al^{3\oplus}$ at pH 2-2.5, unlike Zr analogue. This provides a method of separating Zr from Hf. White solid or gel. Cation exchanger. Various hydrates are known.

[12188-73-7]

Medeiros, L.O., *J. Inorg. Nucl. Chem.*, 1966, **28**, 599 (*synth*)
Pajakov, Sw., *Mikrochim. Acta*, 1966, **7**, 51 (*sepn, Zr, Hf*)

IC-003501

C_2O_6Pu

(Oxalato)dioxoplutonium(*VI*)

Plutonium(VI) (*oxalate*) *dioxide. Plutonyl oxalate*

[69492-92-8]

$PuO_2(C_2O_4)$

M 359.0
Obt. as trihydrate.

Trihydrate: [26627-40-7].
Pink to red monoclinic cryst. Sl. sol. H_2O. Undergoes radiolytic redn. at r.t. Isostructural with U, Np analogues.

▷ Dec. explosively at 180° to PuO_2.

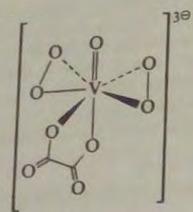
Drobkina, L.Y. *et al*, *Zh. Neorg. Khim.*, 1960, **5**, 805; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1960, **5**, 387 (*soly*)
Jenkins, I.L. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 81.
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, C, 236 (*rev*)
Kalvius, G.M. *et al*, *Phys. Rev. B*, 1978, **18**, 4581.
Kalvius, G.M., *J. Phys. Colloq.*, 1979, 634 (*mössbauer*)

Cleveland, J.M., *The Chemistry of Plutonium*, American Nuclear Society, 1979, 408 (*rev*)
Mefod'eva, M.P. *et al*, *Radiokhimiya*, 1981, **23**, 697 (*cryst struct*)

IC-003502

$C_2O_9V^{3\ominus}$

(Oxalato)oxodiperoxovanadate(*V*)(3−)
[Ethanedioato(2−)-O,O′]oxodiperoxyvanadate(V)(3−), *11Cl.*
Oxalatooxobis(peroxo)vanadate(V)(3−).
Oxobis(peroxo)oxalatovanadate(V)(3−).
Oxalatooxobis(peroxo)vanadate(V)(3−)
[68782-48-9]



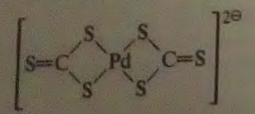
M 218.9 (ion)
Distorted pentagonal bipyramid.
Tri-K salt: [42555-08-8].
Synth. by dissolving V_2O_5 in KOH, adding $H_2C_2O_4$ then H_2O_2 or from KVO_3, $K_2C_2O_4.H_2O$ and $H_2C_2O_4$ in H_2O_2. Bleach for colour film. Orange solid (H_2O). According to Vuletic *et al*, a dihydrate is formed. Schwendt *et al* report that use of $H_2C_2O_4$ yields $K_3[VO(O_2)(C_2O_4)_2]$.
Tri-K salt, monohydrate: [55101-83-2].
Synth. as for the anhydrous salt. Image intensifier for colour film. Orange cryst. It appears that Vuletic *et al* synthesised the monohydrate.
Tri-K salt, mono-H_2O_2 (adduct): [88863-83-6].
Orange cryst. Crystallography shows that this is the correct formulation of the species originally said to be $K_3[V(O_2)_3(C_2O_4)]H_2O$.
Tri-NH_4 salt: [42494-74-6].
Synth. by mixing H_2O_2 solns. of NH_4VO_3 and $(NH_4)_2C_2O_4$. Orange solid (H_2O). According to Vuletic *et al*, a dihydrate is formed.

Vuletic, N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1137 (*synth, ir, K and NH_4 salts*)
Begin, D. *et al*, *Inorg. Chem.*, 1975, **14**, 1785 (*cryst struct, salt, monohydrate*)
Japan. Pat., 77 79 928, (1977); *CA*, **87**, 209509p (*use*)
Japan. Pat., 78 13 418, (1978); *CA*, **89**, 120813b (*use*)
Schwendt, P. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **466**, 232 (*synth, ir, K salt*)
Campbell, N.J. *et al*, *Inorg. Chim. Acta*, 1983, **77**, L215 (*cryst struct, synth, salt, H_2O_2 adduct*)
Djordjevic, C. *et al*, *J. Inorg. Biochem.*, 1985, **25**, 51 (*pharmacol*)
Joniakova, D. *et al*, *Thermochim. Acta*, 1985, **92**, 701 (*thermal dec*)

IC-003503

$C_2PdS_6^{2\ominus}$

Bis(trithiocarbonato)palladate(*II*)(2−)
Bis(carbonotrithioato-S,S′)palladate(2−)



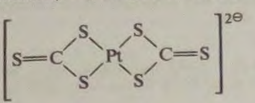
M 322.8 (ion)
Bis-Ph_4As salt: Bright yellow cryst. Sol. $MeNO_2$. Mp 224-225°.

Fackler, J.P. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 3913 (*synth, uv-vis, ir*)

IC-003504

$C_2PtS_6^{2\ominus}$

Bis(trithiocarbonato)platinate(*II*)(2−)
Bis[carbonotrithioato(2−)-S,S′]platinate(II)(2−), *9Cl*



M 411.4 (ion)
Probably square planar. Isomorphous with Ni, Pd analogues. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + $CS_3^{2\ominus}$.
Di-K salt: [73702-29-1].
Bis-Ph_4As salt: [38840-60-7].
Bright orange cryst. ($MeNO_2$/Et_2O). Sol. MeCN, $MeNO_2$. Mp 244-245°.

Fackler, J.P. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 3913 (*synth, ir, uv, struct*)
Burke, J.M. *et al*, *Inorg. Chem.*, 1972, **11**, 2744 (*ir, raman*)

IC-003505

C_2S_2

Ethene-1,2-dithione
Carbon sulfide (C_2S_2)
[83917-77-5]

S=C=C=S

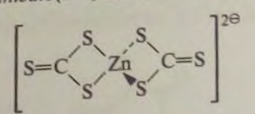
M 88.1
Formed by flash pyrolysis of several S-heterocyclic compds. with matrix isolation. Dec. above 77K to CS. Fairly stable in gas phase at high T and low P.

Maier, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1990, **29**, 1464 (*synth, ir, struct*)
Wentrup, C. *et al*, *J. Am. Chem. Soc.*, 1991, **113**, 3130 (*synth, ms, ir, matrix, isol*)

IC-003506

$C_2S_6Zn^{2\ominus}$

Bis(trithiocarbonato-*S,S′*)zincate(2−)
Bis[carbonotrithioato(2−)-S,S′]zincate(2−), *9Cl*



M 281.8 (ion)
Tetrahedral anion.
Bis-Ph_4P salt: [51435-97-3].
Yellow cryst.
Bis-Ph_4As salt: [51435-98-4].
Yellow cryst.

Müller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **401**, 274 (*synth*)
Cormier, A. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 1059 (*ir*)

IC-003507

C_2Ta_2V

Tantalum vanadium carbide (Ta_2VC_2)

Ta_2VC_2

M 436.8
Struct. comprises close-packed metal-layers: the distribution of C is uncertain. Synth. by hot-pressing Ta and VC in graphite dies. Not completely stoichiometric.

Rudy, E., *J. Less-Common Met.*, 1970, **20**, 49 (*synth, cryst struct*)

IC-003508

C_2UV

Uranium vanadium carbide (UVC_2), 9Cl
[12373-40-9]

UVC_2

M 312.9
Isostructural with $UMoC_2$. Synth. by arc-melting the components under Ar. Dec. to UC and VC above 1900°.

Spear, K.E. *et al*, *High Temp. Sci.*, 1970, **2**, 176 (*synth, phase diagram, cryst struct*)

IC-003509

$C_3AlF_9O_9S_3$

Aluminium tris(trifluoromethanesulfonate)
Tris(trifluoromethanesulfonato)aluminium
[75562-37-7]

$[Al[OS(O)_2CF_3]_3]_n$

M 474.1
Oligomeric (n = 4 or 5) in CH_2Cl_2. Synth. from $AlCl_3$ or Al_4C_3 and CF_3SO_3H in $CFCl_2CF_2Cl$, or from $AlEt_3$ + CF_3SO_3H at −78°. Catalyst in Friedel-Crafts reactions and alkene polym. White moisture-sensitive high-melting powder. Spar. sol. SO_2, SO_2ClF; Sol. Et_2O, Me_2CO, MeCN, $MeNO_2$, diglyme, CH_2Cl_2.

Collomb, J. *et al*, *Eur. Polym. J.*, 1980, **16**, 1135 (*use*)
Collomb, J. *et al*, *Makromol. Chem. Rapid Commun.*, 1980, **1**, 489 (*use*)
Olah, G.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2560 (*synth, props, use, ir, cmr, F-19 nmr, Al-27 nmr*)

IC-003510

C_3AlN_3

Aluminium cyanide

$Al(CN)_3$

M 105.0
Synth. from AlH_3 + HCN in Et_2O. Isol. as complex with Et_2O. Air- and moisture-sensitive white cryst. (Et_2O). Amorphous $LiAl(CN)_4$ also descr.

Wittig, G. *et al*, *Z. Naturforsch., B*, 1951, **6**, 226 (*synth*)

IC-003511

$C_3AlN_3S_3$

Aluminium isothiocyanate
Tris(thiocyanato-N)aluminium

$Al(NCS)_3$

M 201.2
Synth. from Al foil and $(SCN)_2$ in Et_2O. Reacts with arenes to give SCN- subst. derivs. Complex with Et_2O v. hygroscopic cryst.

Söderbäck, E. *et al*, *Acta Chem. Scand.*, 1954, **8**, 1851 (*synth, use*)

IC-003512

C_3Al_4

Aluminium carbide (Al_4C_3)
[1299-86-1]

Al_4C_3

M 143.9
Carbon has 5 (distorted tbp) or 6 (octahedral) coord.; Al 4 (tetrahedral) coord. Synth. from elements at 1000°. Pale yellow moisture-sensitive cryst. Dissolves in hot H_2O or acids to give CH_4. Dissoc. at 1600° to Al + C. Low conc. Al_2C_2 detected in gas by ms. ΔH_f° −207.3 kJ mol^{-1}.

Stackelberg, M.V. *et al*, *Z. Phys. Chem., Abt. B*, 1934, **27**, 37; *Z. Phys. Chem., Abt. A*, 1935, **175**, 127 (*synth, struct*)
Chupka, W.A. *et al*, *J. Phys. Chem.*, 1958, **62**, 611 (*ms*)
Meschi, D.J. *et al*, *J. Phys. Chem.*, 1959, **63**, 1175 (*synth, sp*)
Jeffrey, G.A. *et al*, *Acta Crystallogr.*, 1963, **16**, 559; 1966, **20**, 538 (*cryst struct*)
Cox, J.H. *et al*, *Can. J. Chem.*, 1963, **41**, 1414 (*powder struct*)
Blachnik, R.O.G. *et al*, *Trans. Faraday Soc.*, 1970, **66**, 1038 (*synth, thermodyn data*)
Haworth, D.T. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1689 (*rev*)

C_3AsN_3

Arsinetricarbonitrile, 9Cl
Arsenic cyanide. Tricyanoarsine. Tricyanoarsenic(III). Arsenous tricyanide
[1115-98-6]

IC-003513

$As(CN)_3$

M 152.9
Interatomic distances: As—C 182-196, C—N 113-119 pm; angles: CAsC 87.6-91.5°, AsCN 168-175°. V hygroscopic white, needle-like cryst. Insol $CHCl_3$, CCl_4, Et_2O, MeCN, $AsCl_3$, Subl. 200° in vacuo.
Emersen, K. *et al*, *Acta Crystallogr.*, 1963, **16**, 113 (*synth, cryst struct*)
Miller, F.A. *et al*, *Spectrochim. Acta*, 1965, **21**, 775 (*synth, ir, raman*)
Cyvin, S.J. *et al*, *J. Mol. Struct.*, 1973, **17**, 371 (*struct*)
Edwards, H.G.M. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 733; 1987, **43**, 1345 (*synth, raman*)

$C_3AsN_3O_3$

Arsenous triisocyanate, 9Cl
Arsenic isocyanate, 8Cl. Tris(cyanato-N)arsenic(III)
[4756-58-5]

IC-003514

$As(NCO)_3$

M 200.9
Synth. from $AsCl_3$ + Ag or Na isocyanate. Colourless cryst. (C_6H_6). Mp 97° (94°). Bp 224°.
Gmelin Handbook Inorg. Chem., Syst. No. 17, 1952, 468.
U.K. Pat., 931 240, (1963); *CA*, **59**, 8384 (*synth*)

$C_3AsN_3S_3$

Arsenous trisothiocyanate, 11Cl
Arsenic isothiocyanate, 8Cl. Tris(thiocyanato-N)arsenic(III)
[93383-96-1]

IC-003515

$As(NCS)_3$

M 249.1
Synth. by isom. of the trithiocyanate in MeCN. White cryst. Dec. at r.t. Sol. CS_2, Et_2O, C_6H_6, $CHCl_3$
Sowerby, D.B., *J. Inorg. Nucl. Chem.*, 1961, **22**, 205 (*synth, ir, raman, props*)
Roesky, H.W. *et al*, *Chem. Ber.*, 1985, **118**, 2396 (*reaction*)

C_3BN_3

Boron cyanide ($B(CN)_3$)
Boron tricyanide. Boranetricarbonitrile, 9Cl
[5731-85-1]

IC-003516

$B(CN)_3$

M 88.8
Colourless cryst. Spar. sol. C_6H_6, Et_2O, $CHCl_3$, CS_2. Mp 146.5°.
▷ V. toxic (evolves HCN on contact with moisture).

Chaigneau, M., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1954, **239**, 1220 (*synth*)
Guyes, J., *Bull. Soc. Chim. Fr.*, 1956, 257 (*ir*)

IC-003517

$C_3BN_3O_3$
Boron isocyanate ($B(NCO)_3$)
Boron tris(isocyanate). Triisocyanatoborane, 9CI
[4756-61-0]

$B(NCO)_3$

M 136.8
Unstable colourless gas.
Lappert, M.F. *et al, Adv. Inorg. Chem. Radiochem.*, 1966, **9**, 133 (*rev*)
Alaee, M. *et al, J. Chem. Soc., Dalton Trans.*, 1990, 1569 (*synth, pe*)

IC-003518

$C_3BN_3S_3$
Boron thiocyanate ($B(NCS)_3$)
Tri(isothiocyanato)borane, 9CI, 8CI. Boron trithiocyanate
[44904-18-9]

$B(NCS)_3$

M 185.0
Evidence exists for B—N bonded groups. Colourless liq. Mp −46°. $Bp_{0.5}$ 64-67°.
Sowerby, D.B., *J. Am. Chem. Soc.*, 1962, **84**, 1831 (*synth, ir*)
Dazord, J. *et al, Can. J. Chem.*, 1976, **54**, 2135 (*synth, ms*)
Nöth, H. *et al, NMR Spectroscopy of Boron Compounds (NMR Basic Principles and Progress*, Springer-Verlag, Berlin, 1978 (*B-11 nmr*)
Atchekzai, H.-R. *et al, Can. J. Chem.*, 1979, **57**, 1122 (*synth, B-11 nmr, cmr*)

IC-003519

C_3BrIrO_3
Bromotricarbonyliridium
[17836-58-7]

$[IrBr(CO)_3]_n$

M 356.1
Polymeric. Useful starting material for iridium bromocarbonyl complexes. Cryst. One-dimensional conductor.
Malatesta, L. *et al, J. Inorg. Nucl. Chem.*, 1961, **19**, 81 (*synth*)
Canziani, F. *et al, Chim. Ind. (Milan)*, 1967, **49**, 469 (*synth, use*)

IC-003520

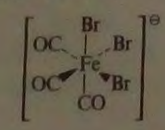
C_3BrO_3Rh
Bromotricarbonylrhodium, 9CI
Bromotris(carbonyl)rhodium
[40784-46-1]

$Rh(CO)_3Br$

M 266.8
Unstable in the absence of a high CO pressure. Ir ν_{CO} 2093, 2054 cm^{-1} (hexane).
Morris, D.E. *et al, J. Organomet. Chem.*, 1973, **49**, C53 (*synth, ir*)

IC-003521

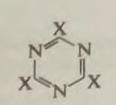
$C_3Br_3FeO_3^{\ominus}$
Tricarbonyltribromoferrate(*II*)(1 −)



M 379.5 (ion)
fac-Octahedral.
K salt: [62048-73-1].
Brown-red cryst. (CH_2Cl_2/Et_2O). Sol. CH_2Cl_2, THF.
Cs salt: [62048-60-6].
Brown-red cryst. (CH_2Cl_2/Et_2O). Sol. CH_2Cl_2, THF.
Pańkowski, M. *et al, J. Organomet. Chem.*, 1977, **125**, 231 (*synth, ir*)

IC-003522

$C_3Br_3N_3$
2,4,6-Tribromo-1,3,5-triazine
Cyanuric bromide
[14921-00-7]

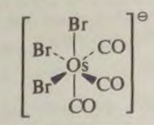


X = Br

M 317.7
Formed by catalysed polym. of BrCN. Cryst., rapidly hydrol. by H_2O. Mp 264°.
Perret, A. *et al, Bull. Soc. Chim. Fr.*, 1940, **7**, 743 (*synth*)
Sawodny, W. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 1327 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 287 (*bibl*)

IC-003523

$C_3Br_3O_3Os^{\ominus}$
Tribromotricarbonylosmate(1 −), 9CI



fac-form

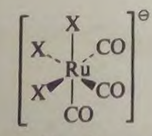
M 513.9 (ion)
Cs salt: [18400-28-7].
$C_3Br_3CsO_3Os$ M 646.8
White cryst. (EtOH).

fac-form
Tetrabutylammonium salt: [58800-94-5].
White.

mer-form
Tetrabutylammonium salt: [58776-23-1].
Bright-yellow.
Cleare, M.J. *et al, J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Preetz, W. *et al, J. Organomet. Chem.*, 1976, **104**, 79 (*synth, ir, raman*)

IC-003524

$C_3Br_3O_3Ru^{\ominus}$
Tribromotricarbonylruthenate(1 −), 9CI, 8CI
[32423-82-8]



X = Br

M 424.8 (ion)
Cs salt: [22594-82-7].
$C_3Br_3CsO_3Ru$ M 557.7
V. pale-yellow cryst.
Cleare, M.J. *et al, J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Colton, R. *et al, Aust. J. Chem.*, 1971, **24**, 903 (*synth, ir*)

$C_3Ca_2Na_2O_9$
Calcium sodium carbonate ($Ca_2Na_2(CO_3)_3$) IC-003525
Carbonic acid, calcium sodium salt (3:2:2), 8CI. Disodium dicalcium carbonate ($Na_2Ca_2(CO_3)_3$). Sodium calcium carbonate
[77403-51-1]

$Na_2Ca_2(CO_3)_3$

M 306.1
Synth. by pptn. from aq. solns. containing stoichiometric amounts of Na_2CO_3 and $CaCO_3$ (1:2). Can be used for the generation of laser light. Colourless to pale yellow orthorhombic cryst. with a vitreous lustre. Pyroelectric. Dec. on heating with evolution of CO_2.
Mineral-form [24492-43-1]
Shortite
Wedge-shaped colourless to yellow cryst.
Adler, H.H. *et al, Am. Mineral.*, 1963, **48**, 839 (*ir*)
Dickens, B., *J. Res. Natl. Bur. Stand. (U.S.), Sect. A*, 1971, **75**, 129 (*cryst struct*)
Frankis, E.J. *et al, Nature (London)*, 1973, **246**, 124 (*synth*)
Meisner, L.B., *Opt. Spektrosk.*, 1981, **50**, 412 (*uses*)

$C_3CdHg_3I_5N_3Se_3$
Pentaiodotris(selenocyanato)trimercurycadmium IC-003526
[12542-44-8]

$Hg_3CdI_5(SeCN)_3$

M 1663.6
Contains bridging SeCN groups. Cryst.
Czakis-Sulikowska, M., *Pol. J. Chem. (Rocz. Chem.)*, 1970, **44**, 1571 (*synth, ir*)

$C_3CdN_3^{\ominus}$
Tris(cyano-*C*)cadmate(1 −) IC-003527
[15698-71-2]

$[Cd(CN)_3]^{\ominus}$

M 190.4 (ion)
Various $R_4P^{\oplus}$ salts have been prepd. from $CdSO_4$ + KCN in the presence of a phosphonium salt.
[73338-45-1, 73338-60-0, 73338-61-1, 73338-62-2]
Papp, S. *et al, Z. Anorg. Allg. Chem.*, 1979, **458**, 241 (*synth, ir*)

$C_3CdN_3Se_3^{\ominus}$
Tris(selenocyanato)cadmate(1 −) IC-003528
[18041-35-5]

$[Cd(SeCN)_3]^{\ominus}$

M 427.3 (ion)
K salt: [26024-27-1].
Prepd. from $CdBr_2$ + KSeCN. Colourless cryst. (Me_2CO). Prac. insol. MeOH, EtOH; sol. H_2O, Me_2CO.
Golub, A.M. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 279 (*synth*)
Tsintsadze, G.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1211 (*ir*)

$C_3CeF_9O_9S_3$
Cerium(*III*) trifluoromethanesulfonate IC-003529
Cerium triflate
[76089-77-5]

$Ce(OSO_2CF_3)_3$

M 587.3
Used in manuf. of antiperspirants and in template synth. Forms adducts with various *O*-donor ligands.
Nonahydrate: [67878-30-2].
$C_3H_{18}CeF_9O_{18}S_3$ M 749.4
Colourless cryst. Sol. H_2O, EtOH, MeCN. Prob contains $[Ce(OH_2)_9]^{3+}$ ions.
[85920-50-9]
Roberts, J.E. *et al, Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
U.S. Pat., 4 219 540, (1980); *CA*, 1981, **94**, 36120 (*use*)
Vincentini, G. *et al, J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)
Chatterjee, A., *Bangladesh J. Sci. Ind. Res.*, 1986, **21**, 148; *CA*, 1988, **109**, 83830 (*cryst struct*)
Bellesis, G.H. *et al, J. Appl. Phys.*, 1987, **61**, 3283 (*magnetism*)
Chatterjee, A. *et al, Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)
Smith, P.H. *et al, Inorg. Chem.*, 1988, **27**, 4154 (*reaction*)

$C_3CeN_3S_3$
Cerium(*III*) thiocyanate IC-003530

$Ce(NCS)_3$

M 314.3
Synth. by metathesis. Used in soln. Forms heptahydrate.
Heptahydrate: [102512-21-0]. *Hexaaquatris(thiocyanato-N) cerium(III) hydrate*
Hygroscopic colourless cryst. Contains $Ce(NCS)_3(OH_2)_6$ molecules with one uncoord. H_2O.
Jolin, S., *Bull. Soc. Chim. Fr.*, 1874, **21**, 533 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110 (*synth, ir*)
Zhu, N. *et al, New Front. Rare Earth Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304; *CA*, 1986, **105**, 70454 (*cryst struct*)

$C_3ClFeHgNO_4$
Tricarbonyl(chloromercurio)nitrosyliron, 8Cl IC-003531
[28407-13-8]

$ClHgFe(CO)_3NO$

M 405.9
Unstable, characterised spectroscopically.
Casey, M. *et al, J. Chem. Soc. A*, 1970, 2258 (*synth, ir*)

C_3ClIrO_3
Tricarbonylchloroiridium(*I*) IC-003532
[32594-40-4]

$[IrCl(CO)_3]_n$

M 311.7
Polymeric. Crystals consist of staggered nonequiv. planar $Ir(CO)_3Cl$ molecules stacked forming parallel chains of Ir atoms. Useful starting material for iridium chlorocarbonyl complexes; catalyst for water gas shift reaction. Highly conducting brown-violet needles with metallic lustre. Subl. in CO.
[28700-98-3]
Fischer, E.O. *et al, Z. Naturforsch., B*, 1962, **17**, 774 (*synth*)
Farone, F. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1625 (*use*)
Aderjan, R. *et al, Z. Naturforsch., A*, 1974, **29**, 1367 (*uv*)
Dahl, L.F. *et al, Prog. Inorg. Chem.*, 1976, **20**, 1 (*ms*)
Reis, A.H. *et al, J. Am. Chem. Soc.*, 1977, **99**, 4184 (*synth, cryst struct, bibl*)
Ford, P.C. *et al, Adv. Chem. Ser.*, 1979, **173**, 81 (*use*)

$C_3ClNiO_3^{\ominus}$ IC-003533

Tricarbonylchloronickelate(1 –), 8CI

Chlorotricarbonylnickelate(1 –)

$[Ni(CO)_3Cl]^{\ominus}$ (C_{3v})

M 178.1 (ion)

Catalyst for carbonylation of benzyl chloride and carbonylation with acetylene insertion of acyl halides. Anion stable in air-free soln. even at 70-80°.

Tetrabutylammonium salt: [27116-03-6].
Not stable in the pure state.

Benzyltrimethylammonium salt: [27116-04-7].
Not stable in the pure state.

Cassar, L. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 291 (*synth, ir*)

C_3ClO_3Rh IC-003534

Tricarbonylchlororhodium, 9CI

Chlorotris(carbonyl)rhodium

[37780-59-9]

$Rh(CO)_3Cl$

M 222.3

Catalyst for the polymerisation of propadiene. Unstable in the absence of a high CO pressure. Ir ν_{CO} 2098, 2052 cm^{-1} (hexane).

Scholten, J.P. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1972, **10**, 3067 (*synth, ir, use*)
Morris, D.E. *et al*, *J. Organomet. Chem.*, 1973, **49**, C53 (*synth, ir*)
Scholten, J.P. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1973, **11**, 3205 (*use*)
Rüger, C. *et al*, *J. Prakt. Chem.*, 1975, **317**, 867.

$C_3Cl_3FeGeNO_4$ IC-003535

Tricarbonylnitrosyl(trichlorogermyl)iron, 8CI

[31275-37-3]

$Cl_3GeFe(CO)_3NO$

M 348.8

Yellow cryst. (pentane). Dec. at 71°.

Casey, M. *et al*, *J. Chem. Soc. A*, 1971, 256 (*synth, ir*)

$C_3Cl_3FeNO_4Sn$ IC-003536

Tricarbonylnitrosyl(trichlorostannyl)iron, 8CI

[27776-74-5]

$Cl_3SnFe(CO)_3NO$

M 394.9

Yellow cryst. (pentane). Mp 101° dec.

Casey, M. *et al*, *J. Chem. Soc. A*, 1971, 256 (*synth, ir*)

$C_3Cl_3GeNiO_3^{\ominus}$ IC-003537

Tricarbonyl(trichlorogermyl)nickelate(1 –), 9CI

Trichlorogermylnickelate(1 –) tricarbonyl

$[Ni(GeCl_3)(CO)_3]^{\ominus}$ (C_{3v})

M 321.6 (ion)

Et_4N salt: [53426-17-8].
Orange cryst. (CH_2Cl_2/pentane). Mp 85°. Mod. unstable, even under N_2.

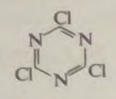
Kruck, T. *et al*, *Z. Naturforsch., B*, 1974, **29**, 198 (*synth*)

$C_3Cl_3N_3$ IC-003538

2,4,6-Trichloro-1,3,5-triazine, 9CI

Cyanuric chloride

[108-77-0]



M 184.4

Known since 1827. Interatomic distances: C—N 133, C—Cl 168 pm; angle: NCN 125°. Synth. from HCN + Cl_2. Commercially available. Used in prepn. of pesticides, herbicides, fungicides, dyestuffs, optical bleaching agents, finishing agents, plastics, explosives, rubber, resins. Reagent for synth. of alkyl halides and deoxygenation of phenols. Cryst. (C_6H_6). Insol. H_2O. Mp 154°. Bp_{720} 190°.

▷ Toxic vapour, irritant, allergen, lachrymator. Exp. carcinogen. Violent reaction with NaOH aq.,DMF, DMSO, MeOH. XZ1400000.

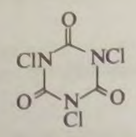
Goubeau, J. *et al*, *J. Phys. Chem.*, 1954, **58**, 1078 (*ir, raman*)
Hoppe, W. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1957, **108**, 321 (*cryst struct*)
Smolin, E.M. *et al*, *Chem. Heterocycl. Compd.*, (Weissberger, A., Ed.), Interscience, N.Y., 1959 (*rev*)
Person, L., *Ind. Chim. (Paris)*, 1966, **53**, 235 (*rev*)
Ross, J.A. *et al*, *Org. Mass Spectrom.*, 1970, **3**, 219 (*ms*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1972, **3**, 72; 1974, **4**, 522; 1975, **5**, 687; 1977, **6**, 149; 1982, **10**, 114 (*uses*)
Geevers, J. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1972, **91**, 331 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 272 (*bibl*)
Sucharda-Sobezyk, A., *Pol. J. Chem. (Rocz. Chem.)*, 1976, **50**, 647 (*ir*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 261.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3342 (*haz, tox*)

$C_3Cl_3N_3O_3$ IC-003539

1,3,5-Trichloro-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione

Trichloroisocyanuric acid, JAN. ***Symclosene,*** *USAN, INN. Trichloroiminocyanuric acid. Chloreal. ACL 85. NSC 405124. ACL 90 Plus*

[87-90-1]



M 232.4

Chlorinating agent, used in pool disinfection products, commercial bleaches and scouring powders; topical disinfectant. Converts ethers to esters. Commercially available. White cryst. Mol. sol. H_2O; sol. chlorinated solvs., v. polar solvs. Mp 248°.

▷ Oxidiser, corrosive; mod. toxic. Potentially explosive with combustible material. Severe irritant. XZ1925000.

Chattaway, F.D. *et al*, *J. Chem. Soc.*, 1902, **81**, 191 (*synth*)
Hands, C.H.G., *Chem. Ind. (London)*, 1948, **67**, 66 (*synth*)
Smolin, E.M. *et al*, *Chem. Heterocycl. Compd.*, Interscience, N.Y. 391, 1959 (*rev*)
Petterson, R.C. *et al*, *J. Org. Chem.*, 1960, **25**, 1595 (*synth, struct*)
Dehmicke, K. *et al*, *Z. Naturforsch., B*, 1971, **26**, 1104 (*ir, raman*)
Gmelin Handbook Inorg. Chem., Syst No 14, 1976, **D3**, 146 (*bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 605 (*use*)

Jeromin, G.E. *et al*, *Chem. Ber.*, 1987, **120**, 649 (*use*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3332 (*haz, tox*)

$C_3Cl_3NiO_3P$ IC-003540

Tricarbonyl(phosphorous trichloride)nickel, 8CI

(Trichlorophosphine)nickel tricarbonyl. Tricarbonyl(trichlorophosphine)nickel. (Phosphorous trichloride)tricarbonylnickel

[18474-97-0]

$Ni(CO)_3PCl_3$ (C_{3v})

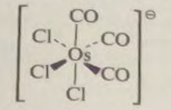
M 280.0

Compound obt. only in soln. Sol. toluene, $CHCl_3$.

Meriwether, L.S. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 3192 (*nmr*)
Tolman, C.A., *J. Am. Chem. Soc.*, 1970, **92**, 2956 (*nmr*)
Bodner, G.M., *Inorg. Chem.*, 1975, **14**, 1932 (*nmr*)

$C_3Cl_3O_3Os^{\ominus}$ IC-003541

Tricarbonyltrichloroosmate(1 –), 9CI



fac-form

M 380.5 (ion)

fac-form

Tetrabutylammonium salt: [58800-92-3].
White cryst. (EtOH).

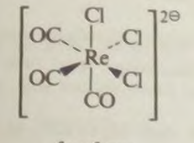
mer-form

Tetrabutylammonium salt: [58755-32-1].
Yellow.

Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Preetz, W. *et al*, *J. Organomet. Chem.*, 1976, **104**, 79 (*synth, ir, raman*)

$C_3Cl_3O_3Re^{2\ominus}$ IC-003542

Tricarbonyltrichlororhenate(2 –), 9CI



fac-form

M 376.5 (ion)

fac-struct predicted by ir.

Di-Cs salt: [35084-05-0].
$C_3Cl_3Cs_2O_3Re$ M 642.4
Synth. from $Re(CO)_5Cl$, HCl, HCOOH and CsCl. Pale yellow cryst. Ir ν_{CO} 2015m, 1885s,br cm^{-1} (KBr).

Bis-Et_4N salt: [25908-19-4].
Synth. from $Re(CO)_5Cl$ and Et_4NCl. White solid. Mp 308-310° dec. Ir ν_{CO} 2000s, 1910s, 1895sh, cm^{-1} (fluorolube); ν_{Re-Cl} 282mw, 241m cm^{-1} (nujol or CsI).

Ginsberg, A.P. *et al*, *Inorg. Chem.*, 1969, **8**, 2189 (*synth, Et_4N salt, ir*)
Colton, R. *et al*, *Aust. J. Chem.*, 1972, **25**, 9 (*synth, Cs salt, ir*)

$C_3Cl_3O_3Ru^{\ominus}$ IC-003543

Tricarbonyltrichlororuthenate(1 –), 9CI, 8CI

[32423-81-7]

As Tribromotricarbonylruthenate(1 –), IC-003524 with

M 291.4 (ion) X = Cl

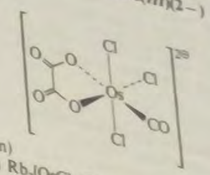
Cs salt: [22594-81-6].
$C_3Cl_3Cs_2O_3Ru$ M 424.3
Pale-yellow cryst. (Me_2CO/pet. ether).

Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Colton, R. *et al*, *Aust. J. Chem.*, 1971, **24**, 903 (*synth, ir*)
Berch, M.L. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 3763 (*synth*)
Teulon, P. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **483**, 219 (*synth*)

$C_3Cl_3O_5Os_2^{2\ominus}$ IC-003544

Carbonyltrichloro(oxalato)osmate(*III*)(2 –)

[83210-36-0]



M 412.5 (ion)

Synth. from $Rb_2[OsCl_5(CO)]$ + KCl and oxalic acid.

Tetrabutylammonium salt: [83210-37-1].
Pale yellow solid.

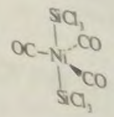
Cs salt: [83210-33-7].
Pale yellow solid.

Schultz, H. *et al*, *J. Organomet. Chem.*, 1982, **235**, 335 (*synth, ir, uv, raman*)

$C_3Cl_6NiO_3Si_2$ IC-003545

Tricarbonylbis(trichlorosilyl)nickel, 10CI

[89377-45-7]



M 411.6

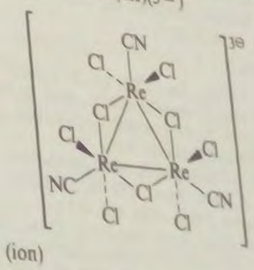
Cryst., stable at 0°, but degrades at r.t. Ir ν_{CO} 2100 cm^{-1}.

Groshens, T.J. *et al*, *J. Organomet. Chem.*, 1983, **259**, 337 (*synth, ir, ms*)
Janikowski, S.K. *et al*, *Organometallics*, 1985, **4**, 397 (*cryst struct*)

$C_3Cl_9N_3Re_3^{3\ominus}$ IC-003548

Tri-μ-chlorohexachlorotricyanorhenate(*III*)(3 –), 8CI

Nonachlorotricyanorhenate(III)(3 –)



M 955.7 (ion)

Tris-Et_4N salt: [22925-07-1].
Synth. from Re_3Cl_9 and Et_4NCN in Me_2CO.
Hygroscopic lilac-coloured solid (Me_2CO).

Gutmann, V. *et al*, *Monatsh. Chem.*, 1969, **100**, 358 (*synth, ir, props*)

C_3Cl_3OU – $C_6IbN_3S_3$

C_3Cl_3OU IC-003547

Pentachloro(2,3,3-trichloro-2-propenyl chloride)uranium(V)

Pentachloro(trichloroethenylchloromethane)uranium(V)

Uranium(V) chloride (2,3,3-trichloro-2-propenyl chloride)

[20576-41-5]

$UCl_5(Cl_2C{=}CClCCl_2)$

M 609.1

Useful starting material for synth. of U(V) complexes. V. moisture-sensitive orange-red cryst. Sol. C_6H_6, CS_2, $SiCl_4$; sl. sol. CCl_4, $CHCl_3$. Mp 145°-146°. μ_{eff} = 1.34μ_B, δ = −1.16. Dec. in H_2O, DMSO.

Selbin, J. *et al*, *Inorg. Chem.*, 1968, **7**, 976 (*synth, use, st-sol*)
Selbin, J. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 3269
Inorg. Synth., 1974, **15**, 243 (*synth*)
Fuji, K. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **42**, 253 (*magnetism, esr*)
Mizuki, C. *et al*, *Inorg. Chim. Acta*, 1989, **165**, 179 (*magnetism*)

$C_2Cl_{10}F_2N_2W_2^{2\ominus}$ IC-003548

[μ-Bis(trifluoromethyl)methylenediimino-*N,N'*] bis(pentachlorotungstate(*IV*))(2−)

*Decachloro[μ-(1,1,2,2,3,3-hexafluoro-2,3-propanediaminato(4−)-*N,N'*)]ditungstate(2−), 10Cl*

$[Cl_5W{=}NC(CF_3)_2N{=}WCl_5]^{2\ominus}$

M 900.2 (ion)

Octahedral at W, short W=N 174.3 pm, W≡N—C unit is nearly linear (176.9°). Formed by unusual reaction of $(F_3C)_2CO$ with W≡N bond.

Bis-Ph_4As salt: [100811-35-6].
Prod. from $(F_3C)_2CO$ + WCl_3N in MeCN with NEt_3 catalyst after addition of $[Ph_4As]Cl$. Orange cryst. (CH_2Cl_2/hexane). Mp 208-210°.

Homsy, N.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 2205 (*cryst struct, synth, ir, F-19 nmr*)

C_3CoNO_4 IC-003549

Tricarbonylnitrosylcobalt, 10Cl, 9Cl, 8Cl

Cobalt tricarbonylnitrosyl

[14096-82-3]

$Co(NO)(CO)_3$

M 172.9

Isoelectric with $[Co(CO)_4]^{\ominus}$. Interatomic distances Co—C 184.3, Co—N 167.1 pm; angles CCoC 111.2°, NCoC 107.7°. Catalyses cyclic oligomerization of acetylenes to benzenes and the dimerization of norbornadiene. Catalyst for the phase-transfer-catalysed carbonylation of benzyl halides. Deep-red liq. Mp −11°. Bp 78.6°. Ir ν 2108, 2046.5, 1822 cm^{-1}.

▷ Probably toxic.

Mond, L. *et al*, *J. Chem. Soc.*, 1922, **121**, 21 (*synth*)
Blanchard, A.A. *et al*, *J. Am. Chem. Soc.*, 1934, **56**, 16 (*synth*)
Brockway, L.O. *et al*, *Trans. Faraday Soc.*, 1937, **33**, 1233 (*ed*)
Inorg. Synth., 1946, **2**, 238 (*synth*)
Bramley, R. *et al*, *J. Chem. Soc. A*, 1967, 861 (*cmr*)
Jones, L.H. *et al*, *J. Chem. Phys.*, 1973, **58**, 3757 (*ir*)
Bor, G., *J. Organomet. Chem.*, 1976, **122**, 413 (*ir*)
Job, R. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1976, **6**, 367 (*synth*)
Schumann, H. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1489 (*nmr, uv*)
Chen, H.W. *et al*, *Inorg. Chem.*, 1979, **18**, 2548 (*pe*)
Hill, J.O. *et al*, *CA*, 1980, **93**, 1786 (*tox*)
Neumann, F. *et al*, *J. Organomet. Chem.*, 1980, **204**, 411 (*nmr*)
Gambarotta, S. *et al*, *J. Organomet. Chem.*, 1981, **212**, C23 (*use*)
Hedberg, K. *et al*, *Inorg. Chem.*, 1985, **24**, 2771 (*ed*)

$C_3CoO_9^{3\ominus}$ IC-003550

Tris(carbonato(2−)-κ*O*,*O'*)cobaltate(*III*)(3−)

Tris(carbonato)cobaltate(III)

$[Co(CO_3)_3]^{3\ominus}$

M 238.9 (ion)

Octahedral complex with bidentate carbonate ligands.

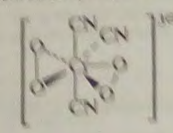
Tris-Na salt, trihydrate: Olive-green powder. Dec. at 93°.

Baxter, H.F., *J. Am. Chem. Soc.*, 1960, **82**, 5031 (*synth*)
Inorg. Synth., 1966, **8**, 202 (*synth*)

$C_3CrN_3O_4^{3\ominus}$ IC-003551

Tris(cyano-*O*peroxychromate(*IV*))(3−), 10Cl

Tris(cyanoperoxochromate(IV))(3−)



M 194.0 (ion)

Pentagonal bipyramidal struct.

Tris-K salt: [65521-60-0].
$C_3CrK_3N_3O_4$ M 311.3
Cryst.

Stomberg, R., *Ark. Kemi.*, 1965, **23**, 401 (*cryst struct*)
Baran, E.J., *Monatsh. Chem.*, 1977, **108**, 1295 (*ir*)

$C_3DyF_9O_9S_3$ IC-003552

Dysprosium(*III*) trifluoromethanesulfonate

Dysprosium triflate

$Dy(OSO_2CF_3)_3$

M 609.7

Forms adducts with various *O*-donor ligands. Affords DyF_3 on pyrolysis.

Nonahydrate: [67878-35-7].
Yellow cryst. Sol. H_2O, EtOH, MeCN. Contains $[Dy(OH_2)_8]^{3\oplus}$ ions.

[85920-56-5]

U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)
Bellesis, G.H. *et al*, *J. Appl. Phys.*, 1987, **61**, 3283, 3286 (*magnetism, esr*)
Chatterjee, A. *et al*, *Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)
Sen, H., *J. Phys. C*, 1988, **21**, 4497 (*magnetism*)

$C_3DyN_3S_3$ IC-003553

Dysprosium(*III*) thiocyanate

$Dy(NCS)_3$

M 336.7

Normally not isol.; synth. metathetically and used as soln.

Hexahydrate: Hygroscopic yellow cryst. Sol. H_2O, EtOH. Presumed 8-coord. by analogy with Eu, Y compds.

Heptahydrate: [38928-02-8].
Yellow cryst. 9-Coord. 3 face capped trigonal prism, with one H_2O uncoord. Contains $Dy(NCS)_3(H_2O)_6$ molecules. Isostructural with Gd-Lu analogues.

Vicentini, G. *et al*, *Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)

Kawamura, K. *et al*, *Trans. Natl. Res. Inst. Met. (Jpn.)*, 1983, **7**, 110 (*ir*)
Lazarev, P.I. *et al*, *Zh. Strukt. Khim.*, 1972, **13**, 580; *J. Struct. Chem. (Engl. Transl.)*, 1972, **13**, 662 (*crystal, cryst struct*)
Lazarev, P.I. *et al*, *Koord. Khim.*, 1975, **1**, 958; *J. Coord. Chem.*, 1975, **1**, 850

$C_3ErF_9O_9S_3$ IC-003554

Erbium(*III*) trifluoromethanesulfonate

Erbium triflate

$Er(OSO_2CF_3)_3$

M 614.4

Forms adducts with various *O*- and *N*-donor ligands. Affords ErF_3 on pyrolysis.

Nonahydrate: [67878-37-9].
Pink cryst. Sol. H_2O, EtOH, MeCN. Prob. contains $[Er(OH_2)_8]^{3\oplus}$ ions.

(*U.S. Pat.*), 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Smirnova, A. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 249 (*synth, ir, complexes*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)
Bellesis, G.H. *et al*, *J. Appl. Phys.*, 1987, **61**, 3286 (*esr*)

$C_3ErN_3S_3$ IC-003555

Erbium(*III*) thiocyanate

$Er(NCS)_3$

M 341.5

Synth. by metathesis and used as soln.

Hexahydrate: Deliquescent pink cryst. Sol. H_2O, EtOH. Presumed 8-coord. by analogy with other lanthanides with one H_2O uncoord.

Cleve, P.T. *et al*, *Bull. Soc. Chim. Fr.*, 1872, **18**, 198 (*synth*)
Vincentini, G. *et al*, *Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al*, *Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*synth, ir*)

$C_3EuF_9O_9S_3$ IC-003556

Europium(*III*) trifluoromethanesulfonate

Europium triflate

[52093-25-1]

$Eu(OSO_2CF_3)_3$

M 599.1

On pyrolysis affords EuF_3. Used in template synth. Forms adducts with various *O* and *N*-donor ligands.

Nonahydrate: [67878-33-5].
Cryst. Sol. H_2O, EtOH, MeCN. Contains $[Eu(OH_2)_9]^{3\oplus}$ ions.

[34629-27-1, 85920-53-2]

U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Massaux, J. *et al*, *Anal. Chim. Acta*, 1974, **73**, 416 (*synth, complex, electrochem*)
U.S. Pat., 3 796 736, (1974); *CA*, 1974, **81**, 13114 (*synth, adducts*)
Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Seminova, A. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 249 (*synth, ir, complexes, fluorescence*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)
Chatterjee, A. *et al*, *Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)
Smith, P.H. *et al*, *Inorg. Chem.*, 1988, **27**, 4154 (*use*)

$C_3EuN_3S_3$ IC-003557

Europium(*III*) thiocyanate

$Eu(NCS)_3$

M 326.2

Synth. by metathesis and used in soln.

Hexahydrate: [102332-24-3].
Colourless cryst. Sol. H_2O. Contains $Eu(NCS)_3(OH_2)_3$ molecules with one H_2O uncoord. Isomorphous with Sm, Gd analogues.

Heptahydrate: Colourless cryst. Isomorphous with other rare earth heptahydrates. Contains $Eu(NCS)_3(OH_2)_4$ molecules.

Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al*, *Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110, 1966, **8**, 10 (*ir*)
Lazarev, P.I. *et al*, *Koord. Khim.*, 1975, **1**, 979; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1975, **1**, 830 (*struct*)
Zhu, N. *et al*, *Acta Pract. Rare Earths Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304, C.A. 1986, **105**, 76634 (*cryst struct*)

$C_3F_3N_3$

2,4,6-Trifluoro-1,3,5-triazine, 9Cl IC-003558

Cyanuric fluoride

M 135.0

Interatomic distances: C—N 133.3, C—F 131.0 pm; angle NCN 127°. Formed from cyanuric chloride + HF or SF_4 or other fluorinating agents. Colourless liq., readily hydrol. d^{20} 1.586. Mp −15°. Bp 72°.

Tullock, W. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 5107 (*synth*)
Ellis, R.L. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 2623 (*pe*)
Schlupf, J. *et al*, *J. Mol. Spectrosc.*, 1975, **54**, 10 (*raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **1**, 226 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 287 (*bib*)

$C_3F_3NiO_3P$ IC-003559

Tricarbonyl(phosphorous trifluoride)nickel, 9Cl, 8Cl

(Trifluorophosphine)nickel tricarbonyl

Tricarbonyl(trifluorophosphine)nickel. (Phosphorus trifluoride)tricarbonylnickel

[14264-32-5]

$Ni(CO)_3PF_3$ (C_{3v})

M 230.6

Colourless, mobile liq. Sol. hexane. d 1.493. Mp −93°. V.p. 88mm at 0°.

Clark, R.J. *et al*, *Inorg. Chem.*, 1965, **4**, 651 (*synth, ir, nmr*)
Bouquet, G. *et al*, *J. Mol. Struct.*, 1968, **1**, 211 (*ir, raman*)
Mathieu, R. *et al*, *Inorg. Chem.*, 1970, **9**, 2030 (*nmr*)
Snow, S.S. *et al*, *Inorg. Chem.*, 1987, **26**, 1597 (*ir*)

$C_3F_3O_3Ru$ IC-003560

Tricarbonyltrifluororuthenium(*III*), 9Cl

[59559-91-0]

$(OC)_3RuF_3$

M 242.0

fac-Octahedral. Synth. by the reaction of Dodecacarbonyltriruthenium, IC-008378 with an excess of XeF_2 in 1,1,2-$C_2Cl_3F_3$ or anhydrous HF at r.t. Buff, air-sensitive solid. $\mu_{eff} = 1.92\mu_B$. Ir ν_{CO} 2148, 2072, ν_{Ru-F} 649, 596 cm^{-1}.

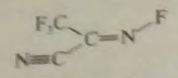
Hewitt, A.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 579 (*synth, ir, esr*)

IC-003561

$C_3F_4N_2$

3,3,3-Trifluoro-2-(fluoroimino)propanenitrile, 12CI

[105882-87-9]



(Z)-form

M 140.0

Formed from N_2F_4 + $F_3CCH{=}CH_2$ at 160°. Colourless liq.

Marsden, H.M. *et al*, *Inorg. Chem.*, 1987, **26**, 169 (*synth, ir, F-19 nmr, ms*)

IC-003562

C_3F_6

Hexafluorocyclopropane, 9CI

Perfluorocyclopropane. Fluorocarbon C-216

[931-91-9]

M 150.0

Gas. Fp −80°. Bp −31.5°.

Haszeldine, R.N., *J. Chem. Soc.*, 1953, 3761 (*synth*)

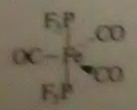
IC-003563

$C_5F_6FeO_3P_2$

Tricarbonylbis(phosphorous trifluoride)iron, 10CI

Tricarbonylbis(trifluorophosphine)iron

[55275-22-2]



trans-form

M 315.8

Exists as a mixt. of 3 rapidly equilibrating isomers. V. volatile yellow liq. Stable in hydrocarbon solvs., rapidly attacked by alcohols, Me_2CO, immisc. H_2O.

Clark, R.J. *et al*, *Inorg. Chem.*, 1964, **3**, 1395 (*synth, ir*)
Ogilvie, F. *et al*, *Inorg. Chem.*, 1969, **8**, 1904 (*nmr*)
Clark, R.J. *et al*, *Acc. Chem. Res.*, 1973, **6**, 248 (*rev*)
Mathieu, R. *et al*, *J. Chem. Phys.*, 1974, **60**, 2997; 1977, **66**, 4822 (*ir, cmr*)
Head, R.A. *et al*, *J. Organomet. Chem.*, 1978, **145**, 75 (*pe*)

IC-003564

$C_5F_6NiO_3Si_2$

Tricarbonylbis(trifluorosilyl)nickel, 10CI

[89377-46-8]

$Ni(CO)_3(SiF_3)_2$

M 312.8

Cryst. Sublimes.

Grosbeux, T.J. *et al*, *J. Organomet. Chem.*, 1983, **259**, 337 (*synth, ir, ms*)

IC-003565

$C_3F_6O_3P_2Ru$

Tricarbonylbis(phosphorous trifluoride)ruthenium, 9CI

Tricarbonylbis(trifluorophosphine)ruthenium(0)

[36429-99-9]

$Ru(CO)_3(PF_3)_2$

M 361.0

Identification only tentative, may be a mixture of isomers. A minor product of the reaction between $Ru_3(CO)_{12}$, CO and PF_3 at 150° and high pressure. Light-yellow liq., identified spectroscopically. Ir ν_{CO} 2082, 2071, 2041, 2026, 2008 cm^{-1} (hexane).

Udovich, C.A. *et al*, *J. Organomet. Chem.*, 1972, **36**, 355 (*synth, ir, nmr*)

IC-003566

$C_3F_9FeO_9S_3$

Iron(*III*) trifluoromethanesulfonate

Ferric trifluoromethanesulfonate. Ferric triflate

[63295-48-7]

$Fe[OS(O)_2CF_3]_3$

M 503.0

Obt. from $FeCl_3$ + CF_3SO_3H. Catalyst for epoxidn. of olefins with iodosylbenzene and oxidative polym. of pyrroles. Photolysis catalyst. White solid.

Haynes, J.S. *et al*, *Can. J. Chem.*, 1981, **59**, 669 (*synth, ir, mössbauer, magnetism*)

IC-003567

$C_3F_9GaO_9S_3$

Gallium(*III*) trifluoromethanesulfonate

Tris(trifluoromethanesulfonato)gallium

[74974-60-0]

$Ga(OSO_2CF_3)_3$

M 516.9

Oligomeric in most solvs. Synth. from GaX_3 (X = Br or Cl) and CF_3SO_3H. Friedel-Crafts catalyst. High melting white solid. Spar. sol. non polar solvs. Sol. diglyme, MeCN, Me_2CO, CH_2Cl_2.

Olah, G.A., *J. Am. Chem. Soc.*, 1988, **110**, 2560.
U.S. Pat., 4 721 559, (1988); *CA*, **109**, 57031 (*use*)

IC-003568

$C_3F_9GdO_9S_3$

Gadolinium(*III*) trifluoromethanesulfonate

Gadolinium triflate

[52093-29-5]

$Gd(OSO_2CF_3)_3$

M 604.4

Affords GdF_3 on pyrolysis.

Nonahydrate: [85920-54-3].
$C_3H_{18}F_9GdO_{18}S_3$ M 766.5
Colourless cryst. Sol. H_2O, EtOH, MeCN. Contains $Gd(OH_2)_9^{3\oplus}$ ions which are tricapped trigonal prismatic. Affords GdF_3 on pyrolysis.

[34629-24-8, 85920-54-3]

Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Harrowfield, J.Mc.B. *et al*, *Aust. J. Chem.*, 1983, **36**, 483 (*synth, cryst struct*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)
Bellesis, G.H. *et al*, *J. Appl. Phys.*, 1987, **61**, 3286 (*esr*)

$C_3F_9HoO_9S_3$

Holmium(*III*) trifluoromethanesulfonate IC-003569

Holmium triflate

$Ho(OSO_2CF_3)_3$

M 612.1

Forms adducts with various *O*- and *N*-donor ligands. Affords HoF_3 on pyrolysis.

Nonahydrate: [67878-36-8].
Yellow cryst. Sol. H_2O, EtOH, MeCN. Contains tricapped trigonal prismatic $[Ho(OH_2)_9]^{3\oplus}$ ions.

U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Seminova, A. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 249 (*synth, ir, complexes, uv-vis*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, ir, complexes*)
Paiva Santos, C.O. *et al*, *Inorg. Chim. Acta*, 1985, **110**, 83 (*synth, cryst struct*)
Sen, H., *J. Phys. C*, 1988, **21**, 4497 (*magnetism*)

$C_3F_9LaO_9S_3$

Lanthanum(*III*) trifluoromethanesulfonate IC-003570

Tris(trifluoromethanesulfonato)lanthanum(III). *Lanthanum triflate*

[52093-26-2]

$La(OSO_2CF_3)_3$

M 586.1

Used in manuf. of antiperspirants, and in template synth. Catalyses range of amine-nitrile reactions.

Nonahydrate: [85920-49-6]. *Nonaaqualanthanum(3+) tris(trifluoromethanesulfonate)*
$C_3H_{18}F_9LaO_{18}S_3$ M 748.2
Colourless needles. Sol. H_2O, EtOH, MeCN. Contains tricapped trigonal prismatic $La(OH_2)_9^{3\oplus}$. Y, Gd, Lu analogues are isomorphous.

[6878-29-9]

Massaux, J. *et al*, *Anal. Chim. Acta*, 1974, **73**, 416 (*polarog*)
Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Seminova, A. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 249 (*synth, ir, adducts*)
U.S. Pat., 4 219 540, (1980); *CA*, 1981, **94**, 36120 (*use*)
Harrowfield, J.Mc.B. *et al*, *Aust. J. Chem.*, 1983, **36**, 483 (*cryst struct*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, adducts*)
Forsberg, J.H. *et al*, *J. Org. Chem.*, 1987, **52**, 1017 (*use*)
Chatterjee, A. *et al*, *Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)
Smith, P.H. *et al*, *Inorg. Chem.*, 1988, **27**, 4154 (*use*)
Forsberg, J.H. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 761 (*use*)

$C_3F_9LuO_9S_3$

Lutetium(*III*) trifluoromethanesulfonate IC-003571

Lutetium triflate

$Lu(OSO_2CF_3)_3$

M 622.1

Affords LuF_3 on pyrolysis.

Nonahydrate: [85920-59-8].
$C_3H_{18}F_9LuO_{18}S_3$ M 784.3
Colourless cryst. Sol. H_2O, EtOH, MeCN. Contains $Lu(OH_2)_9^{3\oplus}$ ions which are tricapped trigonal prismatic.

U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Harrowfield, J.Mc.B. *et al*, *Aust. J. Chem.*, 1983, **36**, 483 (*synth, cryst struct*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)

$C_3F_9NS_3$

Tris(trifluoromethylsulfenyl)amine IC-003572

Nonafluorotrimethylsulfenamide. 1,1,1-Trifluoro-N-N-bis[(trifluoromethyl)thio]methanesulfenamide, 9CI

[4317-00-4]

$(F_3CS)_3N$

M 317.2

Formed from CF_3SNH_2 + CF_3SCl + Me_3N at −60°. Colourless liq. Bp 99.6°.

Haas, A. *et al*, *Chem. Ber.*, 1968, **101**, 3407 (*synth, ir, F-19 nmr, props*)
Haas, A. *et al*, *Z. Anorg. Allg. Chem.*, 1974, **406**, 185 (*reactions*)

$C_3F_9NdO_9S_3$

Neodymium(*III*) trifluoromethanesulfonate IC-003573

Neodymium triflate

[34622-08-7]

$Nd(OSO_2CF_3)_3$

M 591.4

Forms complexes with various *O*- and *N*-donor ligands. On pyrolysis affords NdF_3 and COF_2.

Nonahydrate: [34629-20-4].
Lilac cryst. Sol. H_2O, EtOH, MeCN. Contains tricapped trigonal prismatic $[Nd(OH_2)_9]^{3\oplus}$ ions.

[85920-51-0]

U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436.
U.S. Pat., 3 723 485, (1973); *CA*, 1973, **78**, 147372 (*synth, use*)
Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Seminova, A. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 249 (*synth, ir, uv-vis, complexes*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, adducts*)
Paiva Santos, C.O. *et al*, *Inorg. Chim. Acta*, 1985, **110**, 83 (*synth, cryst struct*)
Chatterjee, A. *et al*, *Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)

$C_3F_9O_9PrS_3$

Praseodymium(*III*) trifluoromethanesulfonate IC-003574

Praseodymium triflate

[52093-27-3]

$Pr(OSO_2CF_3)_3$

M 588.1

Used in template synth. Forms adducts with various *O*-donor ligands. On pyrolysis affords PrF_3.

Nonahydrate: [6878-31-3].
Green cryst. Sol. H_2O, EtOH, MeCN. Contains $[Pr(OH_2)_9]^{3\oplus}$ ions.

[34629-22-6, 85920-51-0]

U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
U.S. Pat., 3 796 736, (1974); *CA*, 1974, **81**, 13114 (*synth, complexes*)
Roberts, J.E. *et al*, *Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Seminova, A. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 249 (*synth*)
Vincentini, G. *et al*, *J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)

Chatterjee, A. *et al, Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)
Smith, P.H. *et al, Inorg. Chem.*, 1988, **27**, 4154 (*use*)
Sen, H., *J. Phys. C*, 1988, **21**, 4497 (*magnetism*)

IC-003575

$C_3F_9O_9S_2Sm$
Samarium(*III*) trifluoromethanesulfonate
Samarium(III) *triflate*
[52093-28-4]

$Sm(OSO_2CF_3)_3$

M 597.5
Pyrolysis affords SmF_3.
Nonahydrate: [67878-32-4]. *Nonaaquasamarium(3+) trifluoromethanesulfonate*
$C_3H_{18}F_9O_{18}S_3Sm$ M 759.7
Yellow cryst. Contains $[Sm(OH_2)_8]^{3\oplus}$ ions.

[34629-23-7, 85920-52-1]
U.S. Pat., 3615169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Massaux, J. *et al, Anal. Chim. Acta*, 1974, **73**, 416 (*electrochem*)
Roberts, J.E. *et al, Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Vincentini, G. *et al, J. Less-Common Met.*, 1983, **94**, 285 (*synth, adducts*)
Chatterjee, A. *et al, Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)

IC-003576

$C_3F_9O_9S_3Tb$
Terbium(*III*) trifluoromethanesulfonate
Terbium(III) *triflate*

$Tb(OSO_2CF_3)_3$

M 606.1
Forms adducts with various *O*- donor ligands.
Nonahydrate: [67913-11-5].
Pale pink cryst. Sol. H_2O, EtOH, MeCN. Contains $[Tb(OH_2)_8]^{3\oplus}$ ions.

[85920-55-4]
U.S. Pat., 3615169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Roberts, J.E. *et al, Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Vincentini, G. *et al, J. Less-Common Met.*, 1983, **94**, 285 (*synth, adducts*)
Bellesis, G.H. *et al, J. Appl. Phys.*, 1987, **61**, 3283 (*magnetism*)
Chatterjee, A. *et al, Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)
Sen, H., *J. Phys. C*, 1988, **21**, 4497 (*magnetism*)

IC-003577

$C_3F_9O_9S_3Tm$
Thulium(*III*) trifluoromethanesulfonate
Thulium triflate

$Tm(OSO_2CF_3)_3$

M 616.1
Forms adducts with various *O*-donor ligands. Affords TmF_3 on pyrol.
Nonahydrate: [74660-76-7].
Green cryst. Sol. H_2O, EtOH, MeCN. Prob. contains $[Tm(OH_2)_8]^{3\oplus}$ ions.

U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Seminova, A. *et al, Inorg. Chim. Acta*, 1980, **40**, 249 (*synth, ir, complexes*)
Vincentini, G. *et al, J. Less-Common Met.*, 1983, **94**, 285 (*synth, complexes*)

$C_3F_9O_9S_3V$ IC-003578
Vanadium(*III*) trifluoromethanesulfonate
Trifluoromethanesulfonic acid, vanadium(III) *salt, 11Cl*
[96332-29-5]

$V(OSO_2CF_3)_3$

M 498.1
Synth. from $V(O_2CCF_3)_3$ and CF_3SO_3H in CF_3COOH.
Green solid. Paramagnetic, $\mu_{eff} = 2.7\mu_B$ (302K).

Sing, S. *et al, J. Fluorine Chem.*, 1985, **27**, 133 (*synth, ir, magnetism, props*)

$C_3F_9O_9S_3Y$ IC-003579
Yttrium(*III*) trifluoromethanesulfonate
Yttrium triflate
[52093-30-8]

$Y(OSO_2CF_3)_3$

M 536.1
Affords YF_3 on pyrolysis.
Nonahydrate: [85920-60-1].
$C_3H_{18}F_9O_{18}S_3Y$ M 698.2
Used in template + other synth. Colourless cryst. Sol. H_2O, EtOH, MeCN. Contains $Y(OH_2)_9^{3\oplus}$ ions which are tricapped trigonal prismatic.

[34629-26-0]
Roberts, J.E. *et al, Thermochim. Acta*, 1978, **25**, 233 (*struct, tga*)
Harrowfield, J.Mc.B. *et al, Aust. J. Chem.*, 1983, **36**, 483 (*synth, cryst struct*)
Vincentini, G. *et al, J. Less-Common Met.*, 1983, **94**, 285 (*struct, adducts*)
Forsberg, J.H. *et al, J. Org. Chem.*, 1987, **52**, 1017 (*use*)
Smith, P.H. *et al, Inorg. Chem.*, 1988, **27**, 4154 (*use*)

IC-003580

$C_3F_9O_9S_3Yb$
Ytterbium(*III*) trifluoromethanesulfonate
Ytterbium triflate
[54761-04-5]

$Yb(OSO_2CF_3)_3$

M 620.2
Used in template synth. Forms complexes with various *O*-donor ligands. Affords YbF_3 on pyrolysis.
Nonahydrate: [67878-38-0].
Colourless cryst. Sol. H_2O, EtOH, MeCN. Prob. contains $[Yb(OH_2)_9]^{3\oplus}$ ions.

[85920-58-7]
U.S. Pat., 3 615 169, (1971); *CA*, 1972, **76**, 5436 (*synth, use*)
Massaux, J. *et al, Anal. Chim. Acta*, 1974, **73**, 416 (*synth, complex, electrochem*)
Roberts, J.E. *et al, Thermochim. Acta*, 1978, **25**, 233 (*synth, tga*)
Vincentini, G. *et al, J. Less-Common Met.*, 1983, **94**, 285 (*synth, complex*)
Chatterjee, A. *et al, Acta Crystallogr., Sect. B*, 1988, **44**, 381 (*cryst struct*)
Smith, P.H. *et al, Inorg. Chem.*, 1988, **27**, 4154 (*use*)

IC-003581

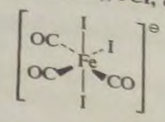
$C_3F_9O_{10}S_3V$
Oxotris(trifluoromethanesulfonato-*O*)vanadium(*V*), 11Cl
[81439-30-7]

$VO(OSO_2CF_3)_3$

M 514.1

Tetrahedral. Synth. from $VOCl_3$ and CF_3SO_3H. Dark green solid. Ir $\nu_{V=O}$ 1005 cm^{-1}.
Sing, S. *et al, J. Fluorine Chem.*, 1985, **27**, 133 (*synth, ir, props*)

$C_3FeI_3O_3^{\ominus}$
Tricarbonyltriiodoferrate(1−), 9CI, 8CI IC-003582



M 520.5 (ion)
fac-Octahedral anion.
K salt: [62048-72-0].
Brown-red. Sol. THF.
Et_4N salt: [20528-31-8].
Synth. from $Fe(CO)_4I_2$ + $[Et_4N]I$. Deep-crimson cryst. Sol. $PhNO_2$. Mp 100° dec.
[62048-71-9]
Chalmers, A.A. *et al, J. Chem. Soc. A*, 1968, 1013 (*synth, ir*)
Pankowski, M. *et al, J. Organomet. Chem.*, 1977, **125**, 231 (*synth, ir*)

$C_3FeNO_4^{\ominus}$
Tricarbonylnitrosylferrate(1−), 9CI, 8CI IC-003583
[15020-24-3]

$[(OC)_3FeNO]^{\ominus}$

M 169.8 (ion)
Starting material for $Fe(CO)_x(NO)$ complexes.
Na salt: [25875-18-7].
$C_3FeNNaO_4$ M 192.8
Air-sensitive yellow cryst. Hygroscopic. Forms yellow needles of addn. compd. (1:1) with 1,4-dioxan.
K salt: [25875-19-8].
C_3FeKNO_4 M 208.9
Bright yellow-orange cryst. (Et_2O/xylene). Sol. THF, Et_2O.
Tl(1+) salt:
C_3FeNO_4Tl M 374.2
Yellow. Sol. CH_2Cl_2. Predominantly ionic.
Me_4N salt: Yellow needles (Me_2CO aq.).
Hieber, W. *et al, Z. Naturforsch., B*, 1960, **15**, 323; 1962, **17**, 323 (*ir, uv*)
Beck, W., *Chem. Ber.*, 1961, **94**, 1214 (*synth*)
Santucci, A. *et al, J. Mol. Struct.*, 1970, **5**, 49 (*ir*)
Casey, M. *et al, J. Chem. Soc. A*, 1971, 256 (*synth, ir*)
Stevens, R.E. *et al, J. Am. Chem. Soc.*, 1981, **103**, 4981 (*synth*)
Pannell, K.H. *et al, Inorg. Chem.*, 1983, **22**, 418 (*cryst struct, ir, nmr*)
Inorg. Synth., 1983, **22**, 165 (*synth*)

$C_3FeN_2O_3^{2\ominus}$
Dicarbonyl(cyano-*C*)nitrosylferrate(2−), 9CI IC-003584

$[(OC)_2Fe(CN)(NO)]^{2\ominus}$

M 167.8 (ion)
Di-K salt: [59060-85-4].
$C_3FeK_2N_2O_3$ M 246.0
Orange.
Bis-Ph_4P salt: [59390-34-0].
Brown cryst.
Nast, R. *et al, Z. Anorg. Allg. Chem.*, 1976, **421**, 15 (*synth, ir*)

$C_3FeN_3O_3^{3\ominus}$
Carbonylbis(cyano-*C*)nitrosylferrate(3−), 9CI IC-003585
$[Fe(CN)_2(CO)(NO)]^{3\ominus}$
M 165.8 (ion)
Struct. not determined.
Tri-K salt: [59060-86-5].
Orange.
Nast, R. *et al, Z. Anorg. Allg. Chem.*, 1976, **421**, 15 (*synth, ir*)

$C_3FeN_3S_3$
Iron(*III*) thiocyanate
Ferric thiocyanate
[4119-52-2] IC-003586

$Fe(SCN)_3$

M 230.0
Only exists under anhydrous conditions. Synth. from: (i) thiocyanogen + iron metal; (ii) slow evap. of soln. of $Ba(NCS)_2$ + $Fe_2(SO_4)_3$; (iii) $Fe(OH)_3$ + HSCN. Difficult to obtain pure. Used to stain samples for electron microscopy; in analytical chem. Dark violet cryst. Sol. H_2O. Forms trihydrate in aq. soln.
Trihydrate: Obt. by crystallisation of $Fe(SCN)_3$ from H_2O. Red cryst. (H_2O).
Schlesinger, H.I. *et al, J. Am. Chem. Soc.*, 1931, **53**, 1212 (*synth*)
Mitchell, K.M. *et al, J. Chem. Soc.*, 1951, 1310 (*synth*)
Sano, H. *et al, Chem. Lett.*, 1973, 43 (*mössbauer, synth*)

$C_3GaN_3S_3$
Gallium(*III*) thiocyanate IC-003587

$Ga(NCS)_3$

M 243.9
Anhydrous compd. not known. Many complexes $Ga(NCS)_3L_3$ with unidentate *N*-donors descr.
Trihydrate: [21991-94-6]. *Triaquatris(isothiocyanato) gallium*(III)
$C_3H_4GaN_3O_6S_3$ M 346.0
Synth. from aq. $Ga_2(SO_4)_3$ + $Ba(NCS)_2$. Pale yellow deliquescent solid. Sol. alcohols, Me_2CO, MeCN, Et_2O. Spar. sol. CH_2Cl_2, cyclohexane, $CHCl_3$. Dec. > 100°. Slow hydrol. in aq. soln.
Patel, S.J. *et al, Can. J. Chem.*, 1969, **47**, 229 (*synth, ir, complexes*)

$C_3GdN_3S_3$
Gadolinium(*III*) thiocyanate IC-003588

$Gd(NCS)_3$

M 331.5
Not usually isol.; prepd. by metathesis and used in soln.
Hexahydrate: [103623-56-9].
Hygroscopic colourless cryst. Contains $Gd(NCS)_3(OH_2)_3$ molecules. 8-coord., with one uncoord. H_2O. Isomorphous with Eu, Sm analogues.
Heptahydrate: Colourless cryst. 9-Coord. with $Gd(NCS)_3(H_2O)_6$ molecules. Isomorphous with some other rare earth heptahydrates.
Sarkar, P.B., *Bull. Soc. Chim. Fr.*, 1926, **39**, 1390 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*ir*)
Lazarev, P.I. *et al, Koord. Khim.*, 1975, **1**, 979; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1975, **1**, 830 (*struct*)

$C_3HCl_2N_3O_3$ – $C_2H_3CuO_4^{\ominus}$

Zhu, N. *et al. New Front. Rare Earth Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304; *CA*, 1988, **105**, 70434 (*cryst struct*)

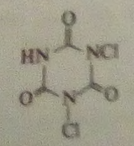
IC-003589

$C_3HCl_2N_3O_3$

1,3-Dichloro-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione, 9CI

Troclosene. Dichloroisocyanuric acid

[2782-57-2]



M 197.9

Chlorinating agent. Topical antiseptic. Cryst. with chlorine odour. Mp 226.4-226.7°.

▷ Severe eye irritant. Emits CO on heating. XZ1845000.

K salt: [2244-21-5]. *Troclosene potassium, USAN, INN. Potassium dichloroisocyanurate, ZAN, ACL 59*

Hygroscopic cryst. Mp 250° dec.

▷ LD_{50} 1215 mg/kg, rat, p.o. XZ1900010.

Na salt: [2893-78-9]. *Aponti-Sterilisierbad. Simple. ACL 60*

▷ XZ1900000.

Petterson, R.C. *et al. J. Org. Chem.*, 1960, **25**, 1595 (*synth, ir*)
Saucier, K.M. *et al. Spectrochim. Acta*, 1964, **20**, 397 (*ir*)
Gottardi, W., *Monatsh. Chem.*, 1970, **101**, 615 (*synth*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 2276.
Kaneto, H. *et al. Oyo Yakuri*, 1984, **27**, 899 (*pharmacol*)
Sax, N.I. *et al. Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1179 (*tox*)

C_3HO_3Ru

IC-003590

Tricarbonyl(hydro)ruthenium(*1-*), 9CI

[54052-34-5]

$[Ru(CO)_3H]_n$

M 186.1

Struct. unknown, prob. polymeric. Isomeric with $[H_4Ru_4(CO)_{12}]$. Insol. from the prolonged reaction between aq. $RuCl_3.xH_2O$ with CO at 80°. Purple-brown, polymeric solid. Insol. org. solvs. Ir ν_{CO} 2000 cm^{-1}.

Rempel, G.L. *et al. Adv. Chem. Ser.*, 1974, **132**, 166 (*synth, ir*)

$C_3HO_{10}Zr^{3\ominus}$

IC-003591

Tris[carbonato(2–)-*O*]hydroxyzirconate(*IV*)(3–), 11CI

Tricarbonato(hydroxy)zirconate(IV)

$[Zr(CO_3)_3OH]^{3\ominus}$

M 288.2 (ion)

Tri-NH_4 salt: [32535-84-5].

$C_3H_{15}N_3O_{10}Zr$ M 342.3

Component of water-repellent treatments for paper and cotton; adhesive in ceramics constructions, used in fire-proofing and rot-proofing cotton, and in diazo-copying material. White solid.

Tri-K salt, trihydrate: [12758-32-6].

Voliotis, C. *et al. Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 1163 (*synth, K salt*)
Trask, B.J. *et al. J. Fire Retard. Chem.*, 1978, **5**, 123 (*use*)
Conner, C.J. *et al. Text. Chem. Color.*, 1978, **10**, 17 (*use*)
Czech. Pat., 206 396, (1983); *CA*, **100**, 94570u (*use*)
Japan. Pat., 85 21 809, (1985); *CA*, **103**, 104440c (*adhesive, use*)
McAlpine, I., *Papier (Darmstadt)*, 1986, **40**, 323 (*use*)

$C_3H_3MnO_4$

IC-003592

(Propanedioato)manganese

Manganese(II)propanedioate. (Malonato)manganese

$[Mn(OOCCH_2COO)]_n$

M 156.9

Synth. by heating the dihydrate. Amorphous solid.

Dihydrate. Diaquat(propanedioato-O,O')manganese

$C_3H_8MnO_6$ M 193.0

Synth. from $MnCO_3$ and aq. malonic acid (10% excess) at 70°. Pale pink cryst. (H_2O). μ_{eff} = 6.00μ_B, high spin Mn(*II*) d^5 complex.

Nagase, K. *et al. Bull. Chem. Soc. Jpn.*, 1975, **48**, 3184 (*synth, ir, tga*)
Liu, T. *et al. Acta Crystallogr., Sect. B*, 1979, **35**, 2212 (*cryst struct, dihydrate*)
Ramade, A.C. *et al. Indian J. Chem.*, 1986, **A, 42** (*magnetism*)

$C_3H_3AlO_6$

IC-003593

Aluminium formate

Tris(formato)aluminium. Normal aluminium formate

[7360-53-4]

$Al(OOCH)_3$

M 162.0

Synth. from $Al(OOCH)_2OH$ + excess HCOOH. Binder and mordant. Used in waterproofing textiles, paper. Amorphous white cryst. + $3H_2O$ (aq. HCOOH).

[22918-74-7]

Donaldson, J.D. *et al. Spectrochim. Acta*, 1964, **20**, 847 (*synth, ir*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 202.

$C_3H_3CdNaO_6$

IC-003594

Cadmium sodium formate ($CdNa(O_2CH)_3$)

Formic acid, cadmium sodium salt (3:1:1)

[77133-53-0]

$CdNa(OOCH)_3$

M 270.4

Octahedral Cd with 6-bridging $HCO_2^{\ominus}$; 2 $HCO_2^{\ominus}$ have 1 O acting as double bridge to form Cd_2O_2 cycle. Cryst. Dec. at 240-280°.

Feliksiński, T. *et al. Mater. Res. Bull.*, 1982, **17**, 627 (*synth, cryst struct, ir*)
Nadzharyan, K.A. *et al. Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 179 (*thermal anal*)
Antsyshkina, A.S. *et al. Koord. Khim.*, 1983, **9**, 418 (*cryst struct*)

$C_3H_3CuO_6^{\ominus}$

IC-003595

Tris(formato-*O*)cuprate(1–), 9CI

Copper(II) formate(1–)

[50928-43-3]

$[Cu(OOCH)_3]^{\ominus}$

M 198.5 (ion)

Octahedral at Cu with extensive formate bridging.

Me_2NH_2 salt: Turquoise cryst.

Sletten, E. *et al. Acta Crystallogr., Sect. B*, 1973, **29**, 1752 (*cryst struct*)

$C_3H_3ErO_6$

Erbium(*III*) formate **IC-003596**

Erbium triformate

[15331-72-3]

$Er(OOCH)_3$

M 302.3

Pink solid. Formed by heating hydrate at 90°.

Dihydrate: [76358-29-7].

Piezoelectric. Square antiprismatic at Er, polymeric struct. Loses H_2O on heating to 90°.

Bis-DMF complex: Cryst. Distorted square antiprismatic. Each Er bound to 2 DMF, 6 bridging formates. Dy analogue also prepd.

[15280-61-2]

Plyushchev, V.E. *et al. Zh. Obshch. Khim.*, 1965, **35**, 1783; *J. Gen. Chem. USSR (Engl. Transl.)*, 1965, **35**, 1781 (*synth*)
Taylor, M.D. *et al. J. Therm. Anal.*, 1974, **6**, 673 (*dta*)
Pabst, A., *Can. Mineral.*, 1978, **16**, 437 (*cryst struct*)
Wenk, H.R., *Z. Kristallogr.*, 1981, **154**, 137 (*cryst struct*)
Fridkin, V.M. *et al. Ferroelectrics*, 1982, **44**, 27; *CA*, **97**, 118936.
Fumanova, N.G. *et al. Kristallografiya*, 1983, **28**, 62; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1983, **28**, 30 (*cryst struct*)
Masuda, Y., *Thermochim. Acta*, 1983, **60**, 203 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. Vol., 1984, **D5**, 5 (*rev, bibl*)
Legendziewicz, J. *et al. J. Less-Common Met.*, 1986, **125**, 45 (*complex, cryst struct, uv-vis*)

$C_3H_3EuO_6$

Europium(*III*) formate **IC-003597**

Europium triformate

[3252-55-9]

$Eu(OOCH)_3$

M 287.0

White cryst. Sol. H_2O.

Phen complex, monohydrate:

$C_{39}H_{33}EuN_6O_7$ M 485.2

Cryst. 8-Coord. Eu bonded to 2N, 4 bridging formates, 1 terminal formate and H_2O.

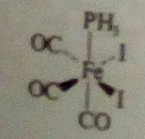
Jamm, C. *et al. J. Am. Chem. Soc.*, 1913, **35**, 754 (*synth*)
Plyushchev, V.E. *et al. Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **160**, 366 (*synth*)
Plyushchev, V.E. *et al. Zh. Strukt. Khim.*, 1966, **7**, 738; *J. Struct. Chem. USSR (Engl. Transl.)*, 1966, **7**, 687 (*struct*)
Grigor'ev, A.I. *et al. Zh. Strukt. Khim.*, 1969, **10**, 48; *J. Struct. Chem. USSR (Engl. Transl.)*, 1969, **10**, 43 (*complex, synth, ir*)
de Hosson, J.T.M. *et al. Spectrochim. Acta, Part A*, 1976, **32**, 1155 (*ir*)
Pabst, A., *Can. Mineral.*, 1978, **16**, 437 (*struct*)
Adamov, L.A. *et al. Koord. Khim.*, 1978, **4**, 1598; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1978, **4**, 149 (*complex, cryst struct*)
Masuda, Y., *Thermochim. Acta*, 1983, **67**, 271 (*tga, dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. Vol., 1984, **D5**, 5 (*rev, bibl*)

$C_3H_3FeI_2O_3P$

IC-003598

Tricarbonyldiiodo(phosphine)iron, 10CI, 8CI

[30003-60-2]



M 427.6

Cryst. (CH_2Cl_2).

Bigorgne, M. *et al. J. Organomet. Chem.*, 1970, **23**, 201 (*synth, ir*)

$C_3H_3GaO_6$

Gallium(*III*) formate **IC-003599**

Gallium trimethanoate. Gallium triformate

$Ga(OOCH)_3$

M 204.7

Synth. from Ga_2O_3 + formic acid. White solid.

Donaldson, J.D. *et al. Spectrochim. Acta*, 1964, **20**, 847 (*synth, ir*)

$C_3H_3GdO_6$

Gadolinium(*III*) formate **IC-003600**

Gadolinium triformate

[3252-56-0]

$Gd(OOCH)_3$

M 292.3

White cryst. Sol. H_2O.

Leipziger, F.D. *et al. Anal. Chem.*, 1964, **36**, 314 (*synth*)
Shklover, C.P. *et al. Zh. Neorg. Khim.*, 1965, **10**, 1121; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 607 (*synth*)
de Hosson, J.T.M. *et al. Spectrochim. Acta, Part A*, 1976, **32**, 1155 (*ir*)
Pabst, A., *Can. Mineral.*, 1978, **16**, 437 (*struct*)
Kistaiah, P. *et al. J. Mater. Sci.*, 1981, **16**, 2321.
Kartha, V. *et al. Spectrochim. Acta, Part A*, 1981, **37**, 927 (*ir, raman*)
Masuda, Y., *Thermochim. Acta*, 1983, **67**, 271 (*dta, fga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. Vol., 1984, **D5**, 5 (*rev, bibl*)

$C_3H_3HoO_6$

Holmium(*III*) formate **IC-003601**

Holmium triformate

[3252-59-3]

$Ho(OOCH)_3$

M 299.9

Yellow solid. Formed by heating hydrate at 90°.

Dihydrate: [76358-27-5].

Yellow cryst. Polymeric struct. with square antiprismatic Ho. Loses H_2O at 80-90°.

[15333-03-6]

Kavedia, C.V. *et al. Indian J. Chem.*, 1970, **8**, 638 (*dta*)
Turcotte, R.P. *et al. J. Solid State Chem.*, 1970, **2**, 593 (*synth*)
Kartha, V.B. *et al. Spectrochim. Acta, Part A*, 1981, **37**, 927 (*ir*)
Wenk, H.R., *Z. Kristallogr.*, 1981, **154**, 137 (*cryst struct*)
Masuda, Y., *Thermochim. Acta*, 1983, **67**, 271 (*dta, fga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. Vol., 1984, **D5**, 5 (*rev, bibl*)

$C_3H_3InO_6$

IC-003602

Indium(*III*) formate

Tris(formato)indium

[40724-25-2]

$In(OOCH)_3$

M 249.8

Synth. from $In(OH)_3$ and HCOOH at 50°. Colourless moisture sensitive solid (HCOOH). Mixed fluoride-formates also descr.

Donaldson, J.D., *Spectrochim. Acta*, 1964, **20**, 847 (*synth, ir*)

Habeeb, J.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 243 (*synth, ir*)
Lindel, W. *et al*, *Z. Anorg. Allg. Chem.*, 1974, **408**, 167 (*synth, ir, ms*)
Opalovskii, A.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 1094 (*related compds*)

IC-003603

$C_3H_3LaO_6$

Lanthanum(*III*) formate
Lanthanum triformate
[2081-11-0]

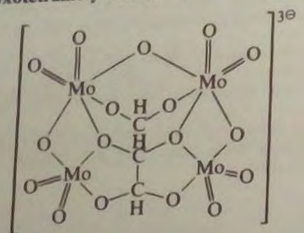
$La(OOCH)_3$

M 273.9
White solid. Sol. H_2O.
de Hosson, J.T.M. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 1155 (*ir*)
Kartha, V.B. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 927 (*ir*)
Masuda, Y., *Thermochim. Acta*, 1983, **67**, 271 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39., *Suppl. Vol.*, 1984, **D5**, 5 (*rev, bibl*)

IC-003604

$C_3H_3Mo_4O_{17}^{3\ominus}$

μ-Formato-μ-glyoxalatopenta-μ-oxooctaoxotetramolybdate(3−)

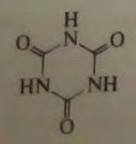


M 694.8 (ion)
Tetranuclear anion. Interatomic distances: Mo-Mo 514.3, 323.1, 367.5 pm.
Day, V.W. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 5971 (*synth*)

IC-003605

$C_3H_3N_3O_3$

Cyanuric acid
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 9CI. Isocyanuric acid. Trihydroxycyanidine
[108-80-5]

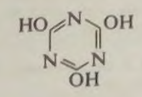


M 129.0
Predominant tautomer; see 1,3,5-Triazine-2,4,6-triol, IC-003606. Depolymerises on heating. Commercially available. Used in rubber, resin manuf. Herbicide. Off-white cryst. + $2H_2O$ (H_2O). Sol. hot EtOH, mod. sol. H_2O. d^0 1.768. Mp >360°. Subl. 380-400°. $Subl._{0.0001}$ 150-180°. pK_a 4.74 (H_2O, 25°). Dec. to cyanic acid on heating without melting. Reacts as mono-, di- or tribasic acid.
▷ Toxic, irritant to skin and eyes. Reacts violently with EtOH. XZ1800000.
1,3-Di-Me: [6726-48-3].
$C_5H_7N_3O_3$ M 157.1
Mp 221-222°.
Tri-N-Me: [827-16-7]. *Trimethyl isocyanurate*
$C_6H_9N_3O_3$ M 171.1
Prisms. Sol. EtOH. Mp 175-176°. Bp 274°.
Tri-N-Et: [715-63-9]. *Triethyl isocyanurate*
$C_9H_{15}N_3O_3$ M 213.2
Prisms. Mp 95°. Bp_{760} 276°.
1,3-Dichloro: see *1,3-Dichloro-1,3,5-triazine-2,4,6(1H,3H,5H)-trione, IC-003589*
Smolin, E. *et al*, *Chem. Heterocycl. Compd.*, 1959, **13**, 20 (*bibl*)
Verschoor, G.C. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 134 (*cryst struct*)
Inorg. Synth., 1972, **13**, 17 (*synth*)
Sucharda-Sobezyk, A., *Pol. J. Chem.* (*Rocz. Chem.*), 1976, **50**, 647 (*ir*)
Kolonko, K.J. *et al*, *J. Org. Chem.*, 1979, **44**, 3769 (*deriv*)
D'Silva, T.D.J. *et al*, *J. Org. Chem.*, 1986, **51**, 3781 (*deriv*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 425, 818.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3312.

IC-003606

$C_3H_3N_3O_3$

1,3,5-Triazine-2,4,6-triol, 9CI
Cyanuric acid



M 129.0
Minor tautomer (with other mixed NH/OH forms) of Cyanuric acid, IC-003605. The synonym Cyanuric acid (and the CAS registry no.) is also applied to the major tautomer. Ethers (cyanuric esters) are hypnotics and anticonvulsants.
Tri-Me ether: [877-89-4].
$C_6H_9N_3O_3$ M 171.1
Mp 135°. Bp 265°.
Tri-Et ether: [884-43-5].
$C_9H_{15}N_3O_3$ M 213.2
Mp 30°. Bp 275°.
Tribenzyl ether:
$C_{24}H_{21}N_3O_3$ M 399.4
Mp 101-102°.
[108-80-5]
Smolin, E.M. *et al*, *Chem. Heterocycl. Compd.*, 1959, **13**, 17 (*rev*)

IC-003607

$C_3H_3O_6Sc$

Scandium(*III*) formate
Scandium triformate
[23405-01-8]

$Sc(OOCH)_3$

M 180.0
6-Coordinate octahedral, polymeric struct. Colourless cryst. Sol. H_2O; sl. sol. hot HCOOH. On heating, dec. to Sc_2O_3 over range 210-400°.
Stěrba-Böhm, J.S. *et al*, *Collect. Czech. Chem. Commun.*, 1935, **7**, 57 (*synth*)
Head, E.L. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 525 (*synth*)
Guseinova, M.K. *et al*, *Zh. Strukt. Khim.*, 1968, **9**, 1040; *J. Struct. Chem. USSR* (*Engl. Transl.*), 1968, **9**, 926 (*cryst struct*)
Arkhangelskii, I.V. *et al*, *Koord. Khim.*, 1977, **3**, 385; *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1977, **3**, 292 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 2 (*rev, bibl*)

$C_3H_3O_6Sn^{\ominus}$

Tris(formato)stannate(*II*)(1−) **IC-003608**

$[Sn(OOCH)_3]^{\ominus}$

M 253.7 (ion)
Synth. from $Sn(OOCH)_2$ and alkali metal or ammonium formate in 40% aq. HCOOH.
K salt: [57763-09-4].
$C_3H_3KO_6Sn$ M 292.8
Cryst. Mp 188-194° dec.
Rb salt: [14567-19-2].
Cryst. Mp 188-194° dec.
Cs salt: [14567-17-0].
Cryst. Mp 152-153°.
NH_4 salt: [14567-22-7].
Cryst. Mp 138-139°.
Donaldson, J.D. *et al*, *J. Chem. Soc.*, 1964, 6107 (*synth*)
Donaldson, J.D. *et al*, *J. Chem. Soc. A*, 1968, 1448 (*mössbauer*)
Donaldson, J.D. *et al*, *Spectrochim. Acta, Part A*, 1969, **25**, 339 (*ir*)

$C_3H_3O_6Tm$

Thulium(*III*) formate **IC-003609**
Thulium triformate
[3118-64-7]

$Tm(OOCH)_3$

M 303.9
Formed from hydrate at 80-90°. Green solid. Sol. HCOOH, H_2O.
Dihydrate: [80495-30-3].
Green cryst. Loses H_2O at 80-90°. Exists in 2 cryst. forms, one form isom. with Yb, Lu analogues, doubly capped trigonal prism; other form prob. square antiprismatic.
[15280-62-3]
Shklover, L.P. *et al*, *Zh. Neorg. Khim.*, 1965, **10**, 1121; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 607 (*synth*)
Kartha, V.S. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 927 (*ir*)
Fermanova, N.G. *et al*, *Kristallografiya*, 1983, **28**, 62; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1983, **28**, 30 (*cryst struct*)
Masuda, Y. *et al*, *Thermochim. Acta*, 1983, **67**, 271 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 5 (*rev, bibl*)

$C_3H_3O_6Y$

Yttrium(*III*) formate **IC-003610**
Yttrium triformate
[15331-71-2]

$Y(OOCH)_3$

M 223.9
White solid. Sol. H_2O. Formed by heating hydrate to 90°.
Dihydrate: [15280-60-1].
Colourless cryst. Polymeric struct. with square antiprismatic Y. Loses H_2O at 80-90°.
[80916-09-2, 80916-10-5, 81809-12-3, 94190-94-0]
Turcotte, R.P. *et al*, *J. Solid State Chem.*, 1970, **2**, 593 (*synth*)
Antsyschkina, A.S. *et al*, *Koord. Khim.*, 1976, **2**, 865; *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1976, **2**, 424 (*cryst struct*)
Wenk, H.R., *Z. Kristallogr.*, 1981, **154**, 137 (*cryst struct*)
Masuda, Y. *et al*, *Thermochim. Acta*, 1983, **60**, 203 (*tga, dga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 5 (*rev, bibl*)

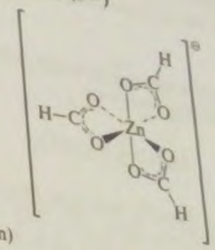
$C_3H_3O_6Yb$

Ytterbium(*III*) formate IC-003611
Ytterbium triformate
[3118-65-8]

M 308.0 $Yb(OOCH)_3$
White solid. Sol. H_2O. Formed by heating hydrate to 90°.
Dihydrate: [85295-28-9].
Colourless cryst. Polymeric struct., dodecahedral or doubly capped trigonal prismatic Yb. Loses H_2O at 80-90°.
[15280-63-4]
Turcotte, R.P. *et al*, *J. Solid State Chem.*, 1970, **2**, 593 (*synth*)
Kartha, V.B. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 927 (*ir*)
Fermanova, N.G. *et al*, *Kristallografiya*, 1983, **28**, 62; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1983, **28**, 30 (*cryst struct*)
Masuda, Y., *Thermochim. Acta*, 1983, **60**, 203 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 5 (*rev, bibl*)

$C_3H_3O_6Zn^{\ominus}$

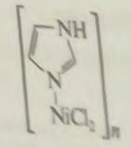
Tris(formato-*O*)zincate(1−) IC-003612



M 200.4 (ion)
Formamidinium salt: [105496-42-2]. *Formamidinium tris(formato)zincate(1−). Tris(formato-O)zincate, hydrogen compd. with methanimidamide (1:1), 11Cl*
$C_4H_8N_2O_6Zn$ M 245.5
Obt. from $ZnCl_2$ in refluxing HCOOH and $HCONH_2$. Cryst. ($HCOOH/HCONH_2$). Struct. comprises 3D-network with 6-coord. Zn (all to O). Erroneously formulated as (Formato-*O*)bis(formamide-*O*)zinc(1+) formate in earlier lit.
[91278-20-5]
Fortier, S. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 1763 (*synth, cryst struct*)
Marsh, R.E., *Acta Crystallogr., Sect. C*, 1986, **42**, 1327 (*synth, cryst struct*)

$C_3H_4Cl_2N_2Ni$

Dichloro(1*H*-imidazole-N^3)nickel(*II*) IC-003613
[28454-39-9]



M 197.6
Polymeric octahedral struct. Pale yellow solid. Mp >300°. μ_{eff} = 3.44μ_B (3.39μ_B).
N-*Me:* [68145-56-2]. *Dichloro(1H-1-methylimidazole-N³)nickel(II)*
$C_4H_6Cl_2N_2Ni$ M 211.7

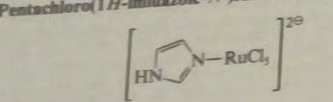
Yellow solid. Polymeric octahedral struct. assigned. μ_{eff} = 3.47 μ_B.

[68145-57-3]

Goodgame, D.M.L. *et al, Inorg. Chem.*, 1968, **7**, 2447 (*synth, ir, raman, uv-vis, magnetism*)
Goodgame, D.M.L. *et al, Inorg. Chim. Acta*, 1969, **3**, 406 (*deriv, synth, ir, uv-vis, magnetism*)
Taylor, C.E. *et al, J. Chem. Soc. A*, 1969, 368 (*synth, magnetism, uv-vis*)
Jansen, J.C. *et al, Z. Naturforsch., B*, 1974, **29**, 527 (*synth, ir, uv-vis*)
Van Dam, J.C. *et al, J. Therm. Anal.*, 1981, **20**, 3 (*iga, deriv*)

$C_3H_4Cl_3N_2Ru^{2\ominus}$ IC-003614

Pentachloro(1*H*-imidazole-*N*^{3})ruthenate(*III*)(2−)



M 346.4 (ion)
Prepd. by treating $RuCl_3.xH_2O$ in aq. HCl with imidazole.
Imidazolium salt: Orange-red cryst.

Krilik, F. *et al, Collect. Czech. Chem. Commun.*, 1961, **26**, 1298.

$C_3H_4N_4O_3Ru$ IC-003615

Diaquatris(cyano-*C*)nitrosylruthenium, 10Cl

Diaquatricyano(nitrosyl)ruthenium

[70699-01-3]

$Ru(NO)(CN)_3(OH_2)_2$

M 245.1
Struct. not known. Prep. by treating $K_4[Ru(CN)_6]$ with aq. HNO_2. Ir ν_{NO} 1927; ν_{CN} 2210, 2160, 2088 cm^{-1}.

Nikol'skii, A.B. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1976, **231**, 622 (*synth, ir*)
Nikol'skii, A.B. *et al, Koord. Khim.*, 1979, **5**, 1851 (*synth*)

$C_3H_5AlCl_4O$ IC-003616

Trichloro(propanoyl chloride)aluminium

[36379-65-4]

$H_3CCH_2C(Cl)=OAlCl_3$

M 225.8
In soln. may be in equilm. with $[H_3CCH_2CO][AlCl_4]$ by analogy with (Acetyl chloride)trichloroaluminium, IC-003040. Synth. from H_3CCH_2COCl and $AlCl_3$. White v. moisture-sensitive cryst. ($SOCl_2$/1,2-dichloroethane). Mp 39-41°.

In Carpenter, J.-M. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 1437 (*synth, ir, cryst struct*)

$C_3H_5HgNO_2S$ IC-003617

(Cysteinato(2−)-*N,O*)mercury

$Hg[SCH_2CH(NH_2)COO]$

M 319.7

Kolthoff, I.M. *et al, Anal. Chim. Acta*, 1961, **24**, 280
Shmitt, H. *et al, J. Am. Chem. Soc.*, 1965, **87**, 1904 (*synth, ir*)
Canty, A.S. *et al, Inorg. Chim. Acta*, 1977, **24**, L77

$C_3H_5NbO_4$ IC-003618

Dioxo(propanoato-*O*)niobium(*V*), 11Cl

[100072-05-7]

$(H_3CCH_2COO)NbO_2$

M 197.9
The products of the reactions between $NbCl_5$ and RCOOH are varied depending on the proportions used and on R. Synth. from $NbCl_5$ and excess propanoic acid in CCl_4. White solid. Ir $\nu_{Nb=O}$ 810 cm^{-1}.

Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1985, **24**, 761 (*synth, ir*)

$C_3H_5O_7Zr^{\ominus}$ IC-003619

Trihydroxy[propanedioato(2−)-*O*]zirconate(*IV*)(1−), 11Cl

Trihydroxymalonatozirconate(IV)(*1*−)

$[OOCCH_2COOZr(OH)_3]^{\ominus}$

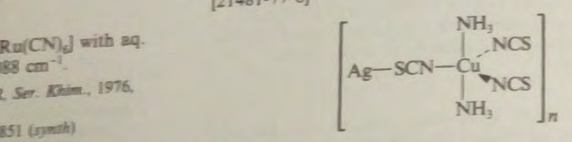
M 244.2 (ion)
Similar salts with other dibasic acids can be isol.
H compd.: [86502-28-5]. (*Hydrogen propanedioato*) *trihydroxyzirconium*(IV). (*Hydrogen malonato*) *trihydroxyzirconium*(IV)
$C_3H_6O_7Zr$ M 245.3
Synth. from $ZrOCl_2$ and malonic acid at pH 2-3 in H_2O.

Belinski, H. *et al, Croat. Chim. Acta*, 1983, **56**, 53 (*synth*)

$C_3H_6AgCuN_5S_3$ IC-003620

Diamminetris(thiocyanato)silver copper

[21481-77-6]



M 379.7
Trigonal bipyramidal at Cu. Bright green cryst. Insol. EtOH, Et_2O.

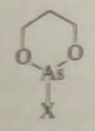
Jin-Ling, H. *et al, Acta Chim. Sin. (Engl. Ed.)*, 1966, **32**, 194 (*cryst struct*)
Slade, R.C. *et al, J. Chem. Soc. A*, 1968, 61 (*synth, esr, uv, magnetism*)
Hathaway, B.J. *et al, J. Chem. Soc. A*, 1970, 806 (*uv, esr*)

$C_3H_6AsClO_2$ IC-003621

2-Chloro-1,3,2-dioxarsenane, 8Cl

2-Chloro-2-arsa-1,3-dioxacyclohexane. Trimethylene chloroarsenite. Trimethylene arsenous chloride

[24630-37-3]



X = Cl

M 184.4
Liq. d_4^{20} 1.79. Bp_{18} 66°, $Bp_{0.1}$ 42°. n_D^{20} 1.5379.

Aksnes, D.W., *Acta Chem. Scand., Ser. A*, 1974, **28**, 1175 (*synth, pmr*)
Kober, F. *et al, Chem. Ber.*, 1976, **109**, 493 (*ms*)
Fuzhev, D.F. *et al, Zh. Obshch. Khim.*, 1976, **46**, 1832; *J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 1776 (*synth, ir*)

Aksnes, D.W. *et al, Acta Chem. Scand., Ser. A*, 1977, **31**, 845; 1981, **35**, 617 (*cmr*)
Zakirev, D.U. *et al, Teor. Eksp. Khim.*, 1977, **13**, 80; *Theor. Exp. Chem. (Engl. Transl.)*, 1977, **13**, 59 (*nqr*)

$C_3H_6AsFO_2$ IC-003622

2-Fluoro-1,3,2-dioxarsenane, 9Cl

2-Fluoro-2-arsa-1,3-dioxacyclohexane. Trimethylene fluoroarsenite. Trimethylene arsenous fluoride

[57915-65-8]

As 2-Chloro-1,3,2-dioxarsenane, IC-003621 with

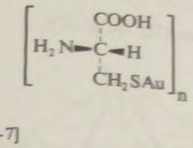
X = F

M 167.9
Liq. Bp_1 37°.

Kober, F. *et al, J. Organomet. Chem.*, 1975, **101**, 57 (*synth*)
Kober, F. *et al, Chem. Ber.*, 1976, **109**, 493 (*ms*)

$C_3H_6AuNO_2S$ IC-003623

(Cysteinato-*O,S*)gold, 10Cl



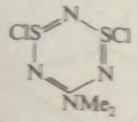
M 317.1
(S)-form [78990-41-7]
L-form
Has poss. role in metab. of Au(I) thiolates used in arthritis therapy. White to pale-yellow light-sensitive solid. V. sol. H_2O, sl. sol. aq. cysteine solns. Mp 180-230°.

Kowala, C. *et al, Aust. J. Chem.*, 1966, **19**, 547 (*synth*)
Danpure, C.J., *Biochem. Pharmacol.*, 1976, **25**, 2343 (*synth*)
Brown, D.H. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 199
Thompson, H.O. *et al, Bioinorg. Chem.*, 1978, **9**, 375 (*rev*)
Shaw, C.F. *et al, Inorg. Perspect. Biol. Med.*, 1979, **2**, 287 (*rev*)
Inorg. Synth., 1982, **21**, 31 (*synth*)

$C_3H_6Cl_2N_4S_2$ IC-003624

1,3-Dichloro-5-(dimethylamino)-1*H*,3*H*-1,3,2,4,6-dithiatriazine

[85869-54-1]



M 233.1
Ring almost planar. Formed by reaction of Me_2NCN + $S_3N_3Cl_3$ in CCl_4 at 65°. Sol. CCl_4.

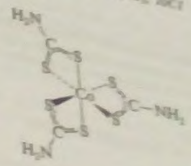
Roesky, H.W. *et al, Z. Naturforsch., B*, 1983, **38**, 347 (*synth, cryst struct*)
Chivers, T. *et al, Inorg. Chem.*, 1986, **25**, 47 (*synth, ir, ms*)

$C_3H_6CoN_3S_6$ IC-003625

Tris(dithiocarbamato)cobalt(*III*) IC-003626

Tris(carbamodithioato-S,S')cobalt(III), 3DCT

[13985-95-0]



M 335.4
Dark green solid.

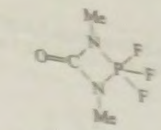
Gahan, L.R., *Inorg. Chem.*, 1979, **18**, 933 (*synth*)

$C_3H_6F_3N_2OP$ IC-003627

2,2,2-Trifluoro-2,2-dihydro-1,3-dimethyl-4-oxa-1,3,2-diazaphosphetidine

2,2,2-Trifluoro-2,2-dihydro-1,3-dimethyl-1,3,2-diazaphosphetidin-4-one, 8Cl

[32707-12-3]



M 174.0
Colourless, fuming liq. Bp_{18} 39°. Dec. during long storage.

Dunmur, R.E. *et al, J. Chem. Soc. A*, 1971, 1289 (*synth, ir, pmr, F-19, P-31 nmr*)
Baldwin, M.A. *et al, Org. Mass Spectrom.*, 1977, **12**, 275 (*ms*)

$C_3H_6HgO_2S$ IC-003627

(Acetato-*O,O'*)(methanethiolato)mercury, 10Cl

(Acetyloxy)(methylmercapto)mercury

[65367-05-7]

MeSHgOAc

M 306.7
Polymeric in solid state with both S and O bridging. Given acidic soln. in H_2O due to partial hydrolysis; sulfur bridging is maintained in aq. soln. Cryst. (H_2O). Sol. H_2O. Mp 133-136°.
Py complex: [66099-21-6]. (Acetato-*O,O'*)(methanethiolato)pyridinemercury, 10Cl
$C_8H_{11}HgNO_2S$ M 385.8
Colourless cryst. Sol. H_2O. Contains infinite chains in solid state. Loses Py at r.t.

Canty, A.J. *et al, Inorg. Chim. Acta*, 1977, **24**, L77 (*synth, spectr, deriv*)
Canty, A.J. *et al, Aust. J. Chem.*, 1978, **31**, 671, 677 (*synth, spectr, deriv, ir, cryst struct*)

$C_3H_6HgO_2Se$ IC-003628

(Acetato)(methaneseleenato)mercury(*II*)

[79790-65-1]

MeSeHgOAc

M 353.6

Prepd. from $Hg(SeMe)_2$ and $Hg(OAc)_2$. Colourless cryst.

Arnold, A.P. *et al, Inorg. Chim. Acta*, 1981, **55**, 171 (*synth, ir, cryst struct*)

IC-003629

$C_3H_6MgO_4$

Methoxy(methyl carbonato-*O*)magnesium, 9CI

Methyl methoxymagnesium carbonate. (Hydrogen carbonato)methoxymagnesium methyl ester, 8CI. Magnesium methyl carbonate

[4861-79-4]

MeOCOOMgOMe

M 130.3

Prepd. by dissoln. of CO_2 in MeOH containing $Mg(OMe)_2$. Commercially available in soln. in DMF (2*M*) or MeOH (0.5*M*). Mild carboxylating agent for nitro and carbonyl compds. Moisture-sensitive; prepd. and used in soln.

▷ Highly toxic, irritant.

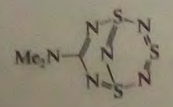
Finkbeiner, H.L. *et al, J. Am. Chem. Soc.*, 1963, **85**, 616 (*synth, uses*)
Whitlock, B.J. *et al, J. Org. Chem.*, 1974, **39**, 3144 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2179D, 2180A (*haz*)

IC-003630

$C_3H_6N_6S_3$

7-(Dimethylamino)-1,3,5-trithia(1,3,5-S^{IV})-2,4,6,8,9-pentaazabicyclo[3.3.1]nona-1(9),2,3,5,7-pentaene

[99618-23-2]



M 222.3

Orange solid.

Chivers, T. *et al, Inorg. Chem.*, 1986, **25**, 272 (*synth, pmr, ir, ms*)

IC-003631

$C_3H_6S_3$

1,3,5-Trithiane, 9CI

s-Trithiane, 8CI. Trithioformaldehyde

[291-21-4]

M 138.2

Reagent for aldehyde synth. *via* carbanion formn. Needles (AcOH). Mp 220°.

▷ YL8225000.

Hexaoxide:

$C_3H_6O_6S_3$ M 234.2

Cryst. powder. Insol. H_2O, org. solvs.; sol. alkalis.

Richtzenhain, H. *et al, Chem. Ber.*, 1953, **86**, 142 (*synth*)
El-Hewehi, Z. *et al, J. Prakt. Chem.*, 1963, **21**, 286 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 564.
Arens, G. *et al, Chem. Ber.*, 1986, **119**, 3631 (*hexaoxide*)
Bencze, Z. *et al, Acta Chem. Scand.*, 1989, **43**, 953 (*struct*)

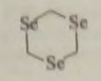
IC-003632

$C_3H_6Se_3$

1,3,5-Triselenane, 9CI

s-Triselenane, 8CI. Trimethylene triselenide. 1,3,5-Triselenacyclohexane

[291-25-8]



M 278.9

Trimer of Selenoformaldehyde, IC-002523. Cryst. Mp 210°, Mp 226-228° (sealed tube).

Bridger, H.J. *et al, J. Chem. Soc.*, 1950, 1371 (*synth*)
Mortillaro, L. *et al, J. Chem. Soc.*, 1965, 807; *J. Polym. Sci., Polym. Chem. Ed.*, 1966, **4**, 248 (*synth*)
Williams, F.D. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 459 (*synth*)
Mammi, M. *et al, Z. Kristallogr.*, 1968, **127**, 401 (*cryst struct*)
Ellestad, O.H. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 149 (*ir, raman*)

IC-003633

$C_3H_7B_3$

Tricarbahexaborane(7), 10CI, 8CI

[23732-88-9]

2,3,4-*carba-form*

M 75.5

nido-. V. unstable at r.t. Formed as mixt. of isomers. Detected by g.l.c. only; methyl derivs. are more stable.

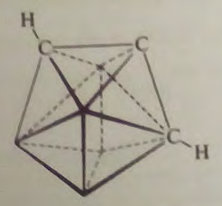
Bramlett, C.L. *et al, J. Am. Chem. Soc.*, 1966, **88**, 4269 (*synth*)

IC-003634

$C_3H_7B_5$

Tricarbaoctaborane(7), 9CI

[11112-28-0]



M 97.1

closo-. Proposed 1,3,7-isomer shown. Air-stable colourless solid. Sol. CS_2. Mp 37°. Pyrolysis at 400° gives $C_2B_5H_7$.

Thompson, M.L. *et al, J. Am. Chem. Soc.*, 1971, **93**, 6677 (*synth, ir, pmr, B-11 nmr, ms*)

IC-003635

$C_3H_7Cl_4NOTi$

Tetrachloro(*N*,*N*-dimethylformamide-*O*)titanium(*IV*), 11CI

Titanium(IV) *chloride dimethylformamide*

[920-29-6]

$(Me_2NCHO)TiCl_4$

M 262.7

Synth. by mixing C_6H_6 solns. of $TiCl_4$ and DMF.

Gerard, W. *et al, J. Chem. Soc.*, 1960, 2141 (*synth*)
Kuz'min, A.I. *et al, Koord. Khim.*, 1982, **8**, 159; *CA*, **96**, 154238o (*Cl-35 nqr*)

IC-003636

$[C_3H_7NO_6P_2Tc^{4\ominus}]$

Dimethylaminomethylenediphosphonate technetium complex

Tc-DMAD. Technetium - DMAD

$[O_3P{-}CH(NMe_2){-}PO_3]^{4\ominus}$ + Tc

Mixt. of ill-characterised species in ratio dependent on synth. conditions. Synth. by $BH_4^{\ominus}$ reduction of $TcO_4^{\ominus}$ in the presence of the ligand. Developed for myocardial infarction imaging and for bone-scanning.

Bell, D. *et al, Br. J. Radiol.*, 1988, **61**, 646 (*pharmacol*)
Holland, M.E. *et al, Nucl. Med. Biol.*, 1989, **16**, 301, 313 (*synth, hplc, biodistribn, pharmacokinetics*)

IC-003637

$C_3H_7NS_2$

Ethyl dithiocarbamate, 8CI

Ethyl carbamodithioate, 9CI. Ethyl aminodithioformate. Dithiourethane

[625-61-6]

M 121.2

Used in ore flotation and in electroplating. Leaflets (Et_2O) with disagreeable odour. Sol. EtOH, Et_2O, insol. H_2O. Mp 41-42°. Dec. on heating above Mp.

N-*Ac: Ethyl acetyldithiocarbamate*

$C_5H_9NOS_2$ M 163.2

Yellow needles (EtOH, H_2O or C_6H_6). Sol. EtOH, Et_2O, hot H_2O. Mp 123-124°.

Delépine, M., *Bull. Soc. Chim. Fr.*, 1903, **29**, 48, 52 (*synth*)
Atkinson, M.R. *et al, J. Chem. Soc.*, 1956, 3847.
U.S. Pat., 2 822 374, (1958); *CA*, **52**, 10147 (*synth*)
Kennard, K.C. *et al, J. Org. Chem.*, 1959, **24**, 464.
Cowen, P.N., *Nature (London)*, 1959, **184**, 366 (*pharmacol*)

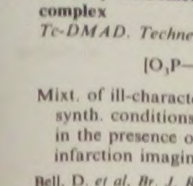
IC-003638

C_3H_8AlN

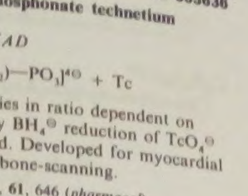
***N*-Isopropyliminoalane**

Hydro[2-propanaminato(2−)]aluminium, 9CI

[44201-48-1]



tetramer



hexamer

R = H
R′ = $CH(CH_3)_2$

M 85.0

Isol. as high polymer, tetramer or hexamer. Catalyst component for stereospecific polymerisation of isoprene and for hydrogenation of alkenes. Reagent for selective redn. of steroidal diketones.

Tetramer: [59120-65-9]. *Tetrahydrotetrakis[μ_3-[2-propanaminato(2−)]]tetraaluminium*
$C_{12}H_{32}Al_4N_4$ M 340.3
White solid.

Hexamer: [53881-02-0]. *Hexahydrohexakis[μ_3-[2-propanaminato(2−)]]hexaaluminium*
$C_{18}H_{48}Al_6N_6$ M 510.5
White solid.

Mazzei, A. *et al, Makromol. Chem.*, 1969, **122**, 168 (*use*)
Cucinella, S. *et al, J. Organomet. Chem.*, 1974, **78**, 185; 1976, **113**, 233 (*synth, ms, pmr, nmr*)
Cesari, M. *et al, J. Organomet. Chem.*, 1974, **78**, 203 (*cryst struct*)
Nöth, H. *et al, Z. Naturforsch., B*, 1976, **31**, 697.
Del Piero, G. *et al, J. Organomet. Chem.*, 1977, **129**, 281 (*cryst struct*)
Paradisi, M.P. *et al, Tetrahedron Lett.*, 1977, 2369 (*use*)
Dozzi, G. *et al, J. Organomet. Chem.*, 1979, **164**, 1 (*use*)

IC-003639

C_3H_8AlN

***N*-Propyliminoalane**

Hydro[1-propanaminato(2−)]aluminium, 9CI

[26534-51-0]

M 85.0

Isol. as high polymer, hexamer or octamer. Struct. of hexamer as *N*-Isopropyliminoalane, IC-003638; struct. of octamer as *N*-Ethyliminoalane, IC-003152, with R = H, R′ = $CH_2CH_2CH_3$.

Hexamer: [57640-77-4]. *Hexahydrohexakis[μ_3-[1-propanaminato(2−)]]hexaaluminium, 9CI*
$C_{18}H_{48}Al_6N_6$ M 510.5

Octamer: [53923-18-5]. *Octahydrooctakis[μ_3-[1-propanaminato(2−)]]octaaluminium, 9CI*
$C_{24}H_{64}Al_8N_8$ M 680.6

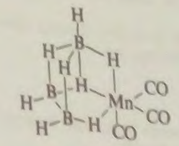
Del Piero, G., *J. Organomet. Chem.*, 1977, **129**, 289 (*cryst struct*)

IC-003640

$C_3H_8B_3MnO_3$

Tricarbonyl[octahydrotriborato(1−)]manganese

[53801-96-0]



M 179.4

Stereochemically non-rigid. Air-sensitive volatile yellow liq. Ir ν_{CO} 2090s, 1990s, 1970w cm^{-1}.

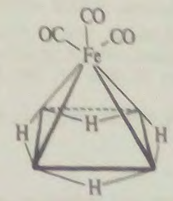
Gaines, D.F. *et al, Inorg. Chem.*, 1978, **17**, 794 (*synth, ir, pmr, ms, B-11 nmr*)
Hildebrandt, J.J. *et al, Inorg. Chem.*, 1978, **17**, 790 (*struct*)
Organomet. Synth., 1988, **4**, 121 (*synth, ir, pmr, B-11 nmr, ms, props*)

IC-003641

$C_3H_8B_4FeO_3$

Tricarbonyl[(1,2,3,4-η)-tetraborane(8)]iron, 10CI

[54748-47-9]



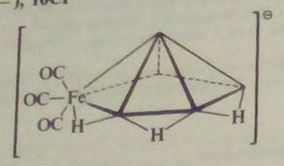
M 191.1

Orange liq. Mp *ca* 5°.

Greenwood, N.N. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 718 (*synth, nmr, pmr, ms, ir*)
Salahub, D.R., *J. Chem. Soc., Chem. Commun.*, 1978, 385 (*pe*)

IC-003642

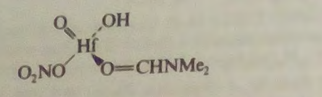
$C_3H_9B_5FeO_3^{\ominus}$
Tricarbonyl[(1,2,5-η)-octahydropentaborato(3−)-H^2]ferrate(1−), 10CI



M 201.9 (ion)
Tetrabutylammonium salt: [61491-75-6].
No phys. props. reported.
Fehlner, T.P. *et al, J. Am. Chem. Soc.*, 1976, **98**, 7085.

IC-003643

$C_3H_9HfN_2O_6$
(*N,N*-Dimethylformamide-*O*)hydroxy(nitrato-*O*)oxohafnium(*IV*), 11CI
[75949-92-7]



M 346.5
Synth. by dissolving $HfO(NO_3)_2$ in dimethyl formamide. Insol. CCl_4.
Kharitonov, Yu.Ya. *et al, Koord. Khim.*, 1980, **6**, 1548; *CA*, **94**, 10546n (*synth, ir*)
Sergushin, N.P. *et al, Koord. Khim.*, 1981, **7**, 808; *CA*, **95**, 33098c (*pe*)
Kharitonov, Yu.Ya. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1109 (*thermal dec*)

IC-003644

$C_3H_8Mg_4O_{14}$
Magnesium carbonate hydroxide hydrate ($Mg_4(CO_3)_3(OH)_2.3H_2O$)
Magnesium tricarbonate dihydroxide trihydrate. Basic magnesium carbonate

$$Mg_4(CO_3)_3(OH)_2.3H_2O$$

M 365.3
Synth. by heating $MgCO_3.3H_2O$ in the presence of ~1% H_2O. White orthorhombic cryst. Dec. on heating with loss of CO_2 and H_2O. Spar. sol. H_2O (0.04 g per 100 cm^3 at 25°; 0.011 g per 100 cm^3 at 100°).
Hydromagnesite [12072-90-1]
Mineral-form
Also formulated as $Mg_5(CO_3)_4(OH)_2.4H_2O$. Widespread occurrence. Colourless or white acicular or bladed cryst.
Fenoglio, M., *Period. Mineral.*, 1936, **7**, 257 (*cryst struct*)
Murdoch, J., *Am. Mineral.*, 1954, **39**, 24 (*cryst struct, mineral*)
Arav, R.I., *Ukr. Khim. Zh.* (*Russ. Ed.*), 1966, **32**, 521; *CA*, **65**, 4992h (*synth*)
Hiroyuki, S. *et al, CA*, 1978, **89**, 190235 (*dta, ir*)

IC-003645

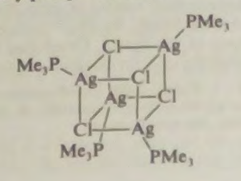
$[C_3H_8N_2O_2Tc]$
2,3-Diaminopropanoic acid technetium complex
Technetium-2,3-diaminopropanoic acid

$$[H_2NCH_2CH(NH_2)CO_2H] + Tc$$

Ill-characterised complex of unknown oxidation state. Synth. from $TcO_4^{\ominus}$ by Sn(*II*) or ascorbate/Fe(*II*) reduction in presence of ligand. Potential radiopharmaceutical use for kidney imaging. Stable in soln. for >1 day.
Chattopadhyay, M. *et al, Nucl. Med. Biol.*, 1987, **14**, 599 (*synth, biodistribn, pharmacokinetics*)

IC-003646

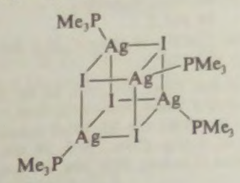
C_3H_9AgClP
Chloro(trimethylphosphine)silver



M 219.3
Tetrameric.
Tetramer: [40696-73-9]. *Tetra-μ_3-chlorotetrakis(trimethylphosphine)tetrasilver, 9CI*
$C_{12}H_{36}Ag_4Cl_4P_4$ M 877.5
Cryst. (C_6H_6/pet. ether). Sol. C_6H_6. Mp 90-92°.
Schmidbaur, H. *et al, Chem. Ber.*, 1972, **105**, 3382 (*synth*)
Schmidbaur, H. *et al, Angew. Chem., Int. Ed. Engl.*, 1973, **85**, 415 (*use*)

IC-003647

C_3H_9AgIP
Iodo(trimethylphosphine)silver



M 310.8
Tetrameric.
Tetramer: [12389-34-3]. *Tetra-μ_3-iodotetrakis(trimethylphosphine)tetrasilver*
$C_{12}H_{36}Ag_4I_4P_4$ M 1243.4
Useful reagent for storing PMe_3. Mp 134-136°. Too unstable for recryst.
Mann, F.G. *et al, J. Chem. Soc.*, 1938, 702 (*synth, use*)
Inorg. Synth., 1967, **9**, 62; 1976, **16**, 153 (*synth, use*)
Pennington, B.T. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 389 (*use*)

IC-003648

$C_3H_9AlCl_3N$
Trichloro(trimethylamine)aluminium
Aluminium trichloride-trimethylamine. Trichloro(N,N′-dimethylmethanamine)aluminium, 9CI
[13869-44-8]

$$Me_3NAlCl_3$$

M 192.4
White moisture-sensitive cryst. Mp 156-157°. Bis-adduct $(Me_3N)_2AlCl_3$ also descr.
Ruff, J.K. *et al, J. Am. Chem. Soc.*, 1961, **83**, 1798 (*synth*)
Sawodny, W. *et al, Z. Phys. Chem.* (*Munich*), 1965, **44**, 227 (*ir, raman*)

Transition Metal Chemistry, Marcel Dekker Inc., N.Y., 1965–

Coordination Chemistry Reviews, Elsevier, 1966–

Inorganic Reaction Mechanisms, Royal Society of Chemistry, London, 1971–

Inorganic Chemistry of the Transition Elements, Royal Society of Chemistry, London, 1972–

Comprehensive Inorganic Chemistry, Trotman-Dickinson, A.F. *et al*, Eds., Pergamon, Oxford, 1973.

Advances in Inorganic Biochemistry, Elsevier, 1977–

Kirk-Othmer Encyclopedia of Chemical Technology, 3rd Edn., Wiley, N.Y., 1978–1984.

Greenwood, N.N. *et al*, *Chemistry of the Elements*, Pergamon, Oxford, 1984.

The Chemistry of the Actinide Elements, 2nd Edn., Katz, J.J. *et al*, Eds., Chapman and Hall, 1986.

Comprehensive Coordination Chemistry, Wilkinson, G. *et al*, Eds., Pergamon, Oxford, 1987.

Cotton, F.A. *et al*, *Advanced Inorganic Chemistry*, 5th Edn., Wiley-Interscience, 1988.

Structures

Wyckoff, R.W.E., *Crystal Structures*, 2nd Edn., Wiley-Interscience, 1963–71.

Wells, A.F., *Structural Inorganic Chemistry*, 5th Edn., Oxford Science, 1984.

Smithells, C.J. *Metals Reference Book*, Plenum Press, N.Y., 1975.

Meyer, W.H., *et al*, *Atlas of Zeolite Structure Types*, 2nd Edn., Butterworths, London, 1987.

International Tables for X-Ray Crystallography, The International Union of Crystallography, London, 1952.

Minerals

Dana, J.D., *System of Mineralogy*, 7th Edn., Wiley, N.Y., 1944.

Encyclopedia of Minerals, 2nd Edn., Roberts, W.I., *et al* Eds., Van Nostrand Reinhold, N.Y., 1990.

Nomenclature

Nomenclature of Inorganic Chemistry, Leigh, G.J. *et al* Eds., IUPAC, Blackwell Scientific, Oxford, 1990.

Synthesis

Brauer, G., *Handbuch Präp. Anorganische Chemie*, 3rd Edn., Ferdinand Enke Verlag, 1975–81.

Inorganic Syntheses, Wiley-Interscience, 1939–

Toxicology

Doull, J. *et al*, *Toxicology*, 3rd Edn., Macmillan, N.Y., 1986.

Grant, D.F. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 377 (*cryst struct*)
Beattie, I.R. *et al*, *J. Chem. Soc. A*, 1969, 2535 (*raman, bis-adduct*)
Almenningen, A. *et al*, *Acta Chem. Scand.*, 1973, **27**, 1821.

$C_3H_9AsO_3$ IC-003649

Trimethyl arsenite, 8CI

Trimethoxyarsine. Arsenous acid trimethyl ester. Trimethoxoarsenic

[6596-95-8]

$As(OMe)_3$

M 168.0
Liq. d_0^{20} 1.43. Bp 129-130°, Bp_{10} 60°. n_D^{20} 1.4402. Easily hydrol.

Inorg. Synth., 1968, **11**, 181 (*synth*)
Lamanova, I.A. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1972, 2675; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1972, 2607 (*ir, raman, deriv*)
Brill, T.B. *et al*, *Inorg. Chem.*, 1973, **12**, 1884 (*synth, ir, nqr*)
Froeyen, P. *et al*, *Org. Mass Spectrom.*, 1973, **7**, 73; 1974, **9**, 132 (*ms, deriv*)
Kober, F. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **403**, 56 (*pmr*)
Preiss, H., *Z. Anorg. Allg. Chem.*, 1974, **404**, 175; *Z. Phys. Chem.* (*Leipzig*), 1976, **257**, 1153 (*ms, deriv*)
Shagidullin, R.R. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1976, **228**, 857; *Dokl. Chem.* (*Engl. Transl.*), 1976, **228**, 395 (*ir, raman, conform*)
Zakirov, D.U. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **235**, 1343; *Dokl. Phys. Chem.* (*Engl. Transl.*), 1977, **235**, 831 (*deriv, nqr*)
Cowley, A.H. *et al*, *Inorg. Chim. Acta*, 1977, **25**, L151 (*pe*)
Baer, C.D. *et al*, *Inorg. Chem.*, 1983, **22**, 1402 (*props*)
Grinberg, E.E. *et al*, *Zh. Fiz. Khim.*, 1986, **60**, 204; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1986, **60**, 116 (*phys props*)
Ando, F. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 1564 (*reactions*)

$C_3H_9AsO_4$ IC-003650

Trimethyl arsenate

Arsenic acid trimethyl ester. Methyl arsenate

[13006-30-9]

$(MeO)_3AsO$

M 184.0
Liq. Bp_{13} 97-99°, Bp_{3-5} 70-75°.

Hass, D., *Z. Chem.*, 1966, **6**, 317 (*synth*)
Vansant, F.K. *et al*, *J. Mol. Struct.*, 1974, **22**, 273 (*ir, raman*)
Froøyen, P. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 132 (*ms*)
Shagidullin, R.R. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1975, 1677; 1977, 1812; (*Engl. transl.* p. 1598, 1672, 1023), 1981, 1289 (*ir, raman, conform*)
Zakirov, D.U. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **235**, 1343; *Dokl. Phys. Chem.* (*Engl. Transl.*), 1977, **235**, 831 (*nqr*)

$C_3H_9BBr_3N$ IC-003651

Tribromo(trimethylamine)boron

Tribromo(N,N-dimethylmethanamine)boron, 10CI. N,N-Dimethylmethanamine compd. with tribromoborane (1:1), 9CI. Trimethylamine compd. with boron bromide (BBr_3) (1:1), 8CI. Boron tribromide trimethylamine. Tribromoborane trimethylamine

[1516-54-7]

$Me_3N—BBr_3$

M 309.6
White cryst. (EtOH or by subl.).

Benton-Jones, B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 2603 (*nmr*)
Van Paasschen, J.M. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1974, **4**, 11 (*synth*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*pmr*)
Miller, J.M. *et al*, *Inorg. Chem.*, 1976, **15**, 284 (*nmr*)
Okuda, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 307 (*nqr, nmr, synth*)
Iijima, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 1908 (*struct*)

$C_3H_9BBr_3P$ IC-003652

Tribromo(trimethylphosphine)boron, 10CI

Trimethylphosphine compd. with tribromoborane (1:1), 9CI. Tribromoborane trimethylphosphine. Boron tribromide trimethylphosphine

[13292-85-8]

$Me_3P—BBr_3$

M 326.6
Solid, dec. at 180°. Mp 255-256° (248°).

Black, D.L. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1116 (*struct*)
Mente, D.C. *et al*, *Inorg. Chem.*, 1975, **14**, 1862 (*nmr, ir, raman, ms*)
Drake, J.E. *et al*, *Inorg. Chem.*, 1977, **16**, 2289 (*ir, raman*)
Sisler, H.H. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1745 (*pmr, synth*)
Apel, J. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **453**, 28.
Iijima, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 2255 (*struct*)

$C_3H_9BCl_3N$ IC-003653

Trichloro(trimethylamine)boron

Trichloro(N,N-dimethylmethanamine)boron, 10CI. N,N-Dimethylmethanamine compd. with trichloroborane (1:1), 9CI. Trimethylamine compd. with boron chloride (BCl_3) (1:1), 8CI. Boron trichloride trimethylamine. Trichloroborane trimethylamine

[1516-55-8]

$Me_3N—BCl_3$

M 176.2
Cryst. (EtOH or by subl.).

Miller, J.M. *et al*, *J. Chem. Soc. A*, 1971, 346 (*ms*)
Benton-Jones, B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 2603 (*nmr*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*pmr*)
Miller, J.M. *et al*, *Inorg. Chem.*, 1976, **15**, 284 (*nmr*)
Okuda, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 307 (*nqr, nmr, synth*)
Iijima, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 1908 (*struct*)

$C_3H_9BCl_3P$ IC-003654

Trichloro(trimethylphosphine)boron, 10CI

Trimethylphosphine compd. with trichloroborane (1:1), 9CI. Trichloroborane trimethylphosphine

[13292-83-6]

$Me_3P—BCl_3$

M 193.2
Cryst. (C_6H_6), stable to heat and water. Mp 241-242°. Subl. 275°.

Phillips, G.M. *et al*, *J. Chem. Soc.*, 1945, 146 (*synth*)
Black, D.L. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1116 (*struct*)
Mente, D.C. *et al*, *Inorg. Chem.*, 1975, **14**, 1852 (*nmr, ms, ir, raman*)
Drake, J.E. *et al*, *Inorg. Chem.*, 1977, **16**, 2289 (*ir, raman*)
Sisler, H.H. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1745 (*pmr, synth*)
Symons, M.C.R. *et al*, *J. Chem. Res. (S)*, 1978, 122.
Apel, J. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **453**, 28 (*nmr*)

IC-003655

$C_3H_9BF_3N$

Trifluoro(trimethylamine)boron

Trifluoro(N,N-dimethylmethanamine)trifluoroboron, 10CI. N,N-Dimethylmethanamine, compd. with trifluoroboranne (1:1), 9CI. Trimethylamine compd. with boron fluoride (BF_3) (1:1), 8CI. Trimethylamine boron trifluoride. Trifluoroborane trimethylamine

[420-20-2]

$Me_3N{-}BF_3$

M 126.9

White cryst. solid. Mp 140-146°. Bp 238°.

Brown, F. *J. Am. Chem. Soc.*, 1952, **74**, 1219 (*synth*)
Miller, J.A. *et al, J. Chem. Soc. A*, 1971, 346 (*ms*)
Clippard, P.H. *et al, J. Cryst. Mol. Struct.*, 1971, **1**, M363 (*cryst struct*)
Van Paasschen, J.M. *et al, J. Am. Chem. Soc.*, 1972, **94**, 2680 (*synth*)
Geanangel, R.A., *Inorg. Chem.*, 1975, **14**, 696 (*cmr, nmr*)
Myers, W.H. *et al, Inorg. Chem.*, 1975, **14**, 2874 (*synth, pmr*)
Miller, J.M. *et al, Inorg. Chem.*, 1976, **15**, 284 (*nmr*)

$C_3H_9BF_3P$

IC-003656

Trifluoro(trimethylphosphine)boron, 10CI

Trifluoroborane trimethylphosphine. Trimethylphosphine compd. with trifluoroborane (1:1), 9CI. Trimethylphosphine compd. with BF_3 (1:1)

[420-21-3]

$Me_3P{-}BF_3$

M 143.8

Solid. Mp 139-142°.

Heitsch, C.W., *Inorg. Chem.*, 1965, **4**, 1019 (*nmr*)
Tuchagues, J.P. *et al, Bull. Soc. Chim. Fr.*, 1971, 4246.
Markham, R.T. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 503 (*synth*)
Bula, M.J. *et al, Can. J. Chem.*, 1975, **53**, 326 (*nmr*)
Van Paasschen, J.M. *et al, Inorg. Chem.*, 1978, **17**, 3302.
Apel, J. *et al, Z. Anorg. Allg. Chem.*, 1979, **453**, 28 (*nmr*)

$C_3H_9BI_3P$

IC-003657

Triiodo(trimethylphosphine)boron, 10CI

Triiodoborane trimethylphosphine. Trimethylphosphine compd. with triiodoborane, 9CI. Trimethylphosphine triiodoborane

[54215-81-5]

$Me_3P{-}BI_3$

M 467.6

Solid, turns light yellow at 125°. Mp 299-302°.

Denniston, M.L. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 1461 (*nmr*)
Black, D.L. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 1116 (*struct*)
Drake, J.E. *et al, Inorg. Chem.*, 1977, **16**, 2289 (*ir, raman*)
Sisler, H.H. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 1745 (*synth, pmr, ir*)
Iijima, K. *et al, Bull. Chem. Soc. Jpn.*, 1982, **55**, 255 (*struct*)

$C_3H_9BN_2$

IC-003658

Cyano(dimethylamine)dihydroboron

(Cyano-C)dihydro(N-methylmethanamine)boron, 10CI. Boranecarbonitrile, compd. with N-methylmethanamine (1:1), 9CI. Cyanoborane dimethylamine

[51329-61-4]

$Me_2NH{-}BH_2CN$

M 83.9

Shows a range of useful pharmacological props. White hygroscopic cryst. solid. Sol. Et_2O. Mp 46-48°, Mp 54-55°.

Weidig, C. *et al, Inorg. Chem.*, 1974, **13**, 1763 (*synth, ir*)
Beachley, O.T. *et al, Inorg. Chem.*, 1975, **14**, 120 (*pmr*)
Wisian-Nielson, P. *et al, Inorg. Chem.*, 1978, **17**, 2327 (*synth, pmr, ir*)
Hall, I.J. *et al, J. Pharm. Sci.*, 1979, **68**, 685; 1980, **69**, 1025; 1981, **70**, 339 (*pharmacol*)

IC-003659

C_3H_9BS

Dimethyl(methylthio)borane

Dimethylthioborinic acid methyl ester, 10CI, 9CI, 8CI

[19163-05-4]

Me_2BSMe

M 87.9

Air- and moisture-sensitive liq., dec. over several months at 20°. Mp −84°. Bp 71°.

Burg, A.B. *et al, J. Am. Chem. Soc.*, 1954, **76**, 3307 (*synth, props*)
Nöth, H. *et al, J. Organomet. Chem.*, 1968, **12**, 23 (*nmr*)
Vahrenkamp, H., *J. Organomet. Chem.*, 1971, **28**, 181 (*raman, ir*)
Kroner, J. *et al, Z. Naturforsch., B*, 1973, **28**, 416 (*pe*)
McFarlane, W. *et al, Chem. Ber.*, 1975, **108**, 3831 (*nmr*)
Berger, H.O. *et al, Chem. Ber.*, 1976, **109**, 2266 (*props*)

$C_3H_9BS_3$

IC-003660

Tris(methylthio)borane

Thioboric acid, trimethyl ester, 10CI, 9CI, 8CI. Tris(methylmercapto)borane

[997-49-9]

$B(SMe)_3$

M 152.1

B—S bonds readily cleaved by protic species and BX_3. Malodorous colourless liq. Sol. aprotic solvs. eg. C_6H_6, ethers. d^{20} 1.098. Mp 4.1-4.9°. Bp_{18} 100°, Bp_2 59°.

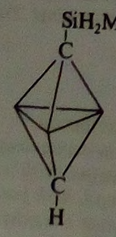
Goubeau, J. *et al, Z. Anorg. Allg. Chem.*, 1952, **270**, 16 (*synth, ir, raman*)
Vahrenkamp, H., *J. Organomet. Chem.*, 1971, **28**, 181 (*ir, raman*)
Cragg, R.H. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1373 (*ms*)
Johansen, R. *et al, Acta Chem. Scand.*, 1973, **27**, 3015 (*ed, gas phase struct*)
Nöth, H. *et al, Chem. Ber.*, 1974, **107**, 3104 (*pmr, B-11 nmr*)
McFarlane, W. *et al, Chem. Ber.*, 1975, **108**, 3831 (*cmr*)

$C_3H_9B_3Si$

IC-003661

1-(Methylsilyl)-1,5-dicarbapentaborane(5), 9CI

[55906-10-0]



M 105.6

Colourless liq. isolated by cold column fractionation between −86° and −90° under high vacuum.

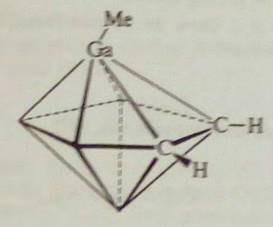
Leach, J.B. *et al, J. Chem. Soc., Dalton Trans.*, 1975, **11**, 1018 (*ir, nmr, ms, synth*)

IC-003662

$C_3H_9B_4Ga$

[(2,3,4,5,6-η)-Hexahydro-2,3-dicarbahexaborato(2−)]methylgallium, 9CI

[36550-13-7]



M 158.0

Colourless, sl. volatile cryst. slowly degraded by air. Stable to 100°.

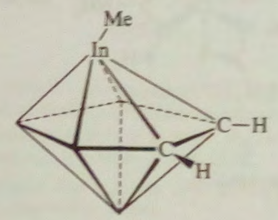
Grimes, R.N. *et al, J. Am. Chem. Soc.*, 1972, **94**, 1865 (*synth, cryst struct, ir, ms, nmr*)

IC-003663

$C_3H_9B_4In$

[(2,3,4,5,6-η)-Hexahydro-2,3-dicarbahexaborato(2−)]methylindium, 9CI

[36550-14-8]



M 203.1

Colourless, sl. volatile cryst. by subl. Struct. by analogy with Ga analogue. Thermally stable to ~100°.

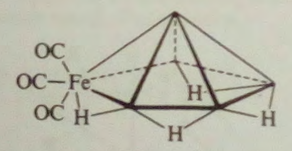
Grimes, R.N. *et al, J. Am. Chem. Soc.*, 1972, **94**, 1865 (*synth, ir, ms, pmr, nmr*)

IC-003664

$C_3H_9B_5FeO_3$

Tricarbonyl[nonahydropentaborato(2−)]iron, 10CI

[61403-41-6]



M 203.0

Fluxional. Deep-red mobile liq.

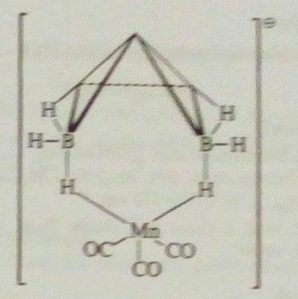
▷ Extremely pyrophoric.

Fehlner, T.P. *et al, J. Am. Chem. Soc.*, 1976, **98**, 7085 (*synth, nmr, ms, pmr, cmr*)
Ulman, J.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 456 (*pe*)
Shore, S.G. *et al, Inorg. Chem.*, 1979, **18**, 670 (*synth, ms, pmr, cmr, nmr*)

IC-003665

$C_3H_9B_5MnO_3^{\ominus}$

Tricarbonyl[nonahydropentaborato(2−)]manganate(1−), 10CI



M 202.0 (ion)

Na salt: [71230-46-1].
Characterised in soln.

Tetrabutylammonium salt: [71230-45-0].
Characterised in soln. Ir ν_{CO} 1990vs, 1920vs, 1900vs cm^{-1} (CH_2Cl_2).

Fischer, M.B. *et al, Inorg. Chem.*, 1979, **18**, 3200 (*synth, ir, pmr, B-11 nmr*)

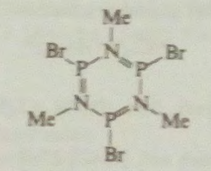
IC-003666

$C_3H_9Br_3N_3P_3$

2,4,6-Tribromo-1,2,3,4,5,6-hexahydro-1,3,5-trimethyl-1,3,5,2,4,6-triazaphosphorine, 10CI

2,4,6-Tribromo-1,3,5-trimethylcyclotriazaphosphane

[70538-66-8]



M 419.7

Solid. Mp 149-150°.

Zeiss, W. *et al, Z. Naturforsch., B*, 1979, **34**, 423, 678 (*synth, pmr, P-31 nmr, reactions*)
Zeiss, W. *et al, Z. Anorg. Allg. Chem.*, 1981, **475**, 256 (*reactions*)

IC-003667

$C_3H_9ClO_9S_3Ti$

Chlorotris(methanesulfonato-*O*)titanium(*IV*), 11CI

[55042-27-8]

$TiCl(OSO_2Me)_3$

M 368.6

Synth. from $TiCl_4$ + $3MeSO_3H$ in pet. ether. Pale yellow solid. Mp >200°.

Paul, R.C. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 1933 (*synth*)

IC-003668

$C_3H_9Cl_2NbO_3$

Dichlorotrimethoxyniobium(*V*), 11CI

[20759-06-2]

$NbCl_2(OMe)_3$

M 256.9

Synth. by heating $NbCl_5$ and MeOH under reflux in C_6H_6. Light coloured, air-sensitive solid. Sol. pet. ether.

Miranda, C. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 839 (*uv-vis*)

$C_3H_9Cl_3NPd^{\ominus}$ – $C_3H_9CrF_{12}N_3P_3$

Kodama, H. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **421**, 71 (*synth, thermal dec*)
Geetha, C.N. *et al*, *Indian J. Chem., Sect. A*, 1985, **24**, 236 (*synth*)

IC-003669

$C_3H_9Cl_3NPd^{\ominus}$

Trichloro(trimethylamine)palladate(*II*)(1−)

$[PdCl_3(NMe_3)]^{\ominus}$

M 271.8 (ion)
Tetrapropylammonium salt: [37084-09-6].
Orange-brown cryst. Sol. Me_2CO, CH_2Cl_2. Mp 106-109° dec. Ir ν_{Pd-Cl} 337, 318-322 cm^{-1}.

Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1298 (*synth, ir, raman*)

IC-003670

$C_3H_9Cl_3NSiV$

Trichloro(trimethylsilylimido)vanadium(*V*)
Trichloro[1,1,1-trimethylsilanaminato(2−)]vanadium(V), *11Cl*
[99589-88-5]

$Me_3SiN{=}VCl_3$

M 244.4
Pseudo-tetrahedral at V. Si—N 179 pm, angle: VNSi 177.5°. Synth. from VCl_3 and Me_3SiN_3 in CCl_4. Volatile, v. moisture-sensitive orange-red solid.

Schweda, E. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **528**, 117 (*synth, cryst struct, ir*)

IC-003671

$C_3H_9Cl_3O_3PPt^{\ominus}$

Trichloro(trimethyl phosphite)platinate(*II*)(1−), 10Cl

$PtCl_3[P(OMe)_3]^{\ominus}$

M 425.5 (ion)
Square planar. Synth. from $[Pt(PX_3)Cl_3]^{\ominus}$ (X = Cl, Br) + MeOH.
Tetrabutylammonium salt: [62428-87-9].
Not isol. Yellow in soln. Sol. CH_2Cl_2.

Crocker, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2494 (*synth, pmr, P-31 nmr, Pt-195 nmr*)
Gosling, R. *et al*, *Inorg. Chem.*, 1983, **22**, 1235 (*reactions*)

IC-003672

$C_3H_9Cl_3PPt^{\ominus}$

Trichloro(trimethylphosphine)platinate(*II*)(1−), 9Cl

$[PtCl_3(PMe_3)]^{\ominus}$

M 377.5 (ion)
Square planar. Synth. from $Pt_2Cl_4(PMe_3)_2$ + $Cl^{\ominus}$. Subject of substitution mechanism studies. Br, I analogues known.
Tetrapropylammonium salt: [19508-36-2].
Yellow solid. Sol. $CHCl_3$, CH_2Cl_2. Mp 145°.

Duddell, D.A. *et al*, *J. Chem. Soc. A*, 1970, 545 (*synth, ir, raman*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1298 (*uv*)
Goggin, P.L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 176 (*Pt-195 nmr*)
Gosling, R. *et al*, *Inorg. Chem.*, 1983, **22**, 1235 (*reactions*)

IC-003673

$C_3H_9Cl_{10}MoP_3$

Tetrachlorotris(methylphosphonous dichloride) molybdenum, 10Cl
Tetrachlorotris[dichloro(methyl)phosphine]molybdenum(IV)
[69039-67-4]

$MoCl_4(PMeCl_2)_3$

M 588.4
7-Coordinate with Cl capping face occupied by three P atoms. Interatomic distances: Mo—P 255.5, Mo—Cl 240.1(x3), 235.4 pm. Air-sensitive dark green cryst. (CS_2). $\mu_{eff} = 2.71\mu_B$ (300K).

Bullock, J.I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1536 (*cryst struct, synth, ir, uv*)

IC-003674

$C_3H_9CoN_6S_6$

Tris(dithiocarbazato)cobalt(*III*), 8Cl
[34195-93-2]

$Co[NH_2NHCS_2]_3$

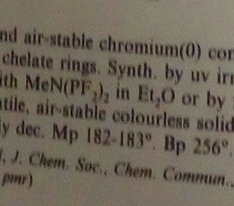
M 380.4
Beige solid.

Battistoni, C. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 1081 (*uv, ir*)

IC-003675

$C_3H_{12}CoN_9S_3$

Tris(thiosemicarbazido)cobalt(*III*)



fac-form

M 326.2

fac-form
Pinkish-lilac needles.

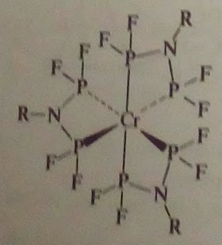
mer-form
Greyish-green solid.

Samus', N.M. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1961, **6**, 1042 (*synth*)
Sun, K.K.W. *et al*, *Can. J. Chem.*, 1970, **48**, 2327 (*synth, uv*)

IC-003676

$C_3H_9CrF_{12}N_3P_6$

Tris[*N*-methylaminobis(difluorophosphine)-*P,P'*] chromium(0)
*Tris(methylimidodiphosphorous tetrafluoride-*P,P')*chromium*, *10Cl*
[63404-40-0]



R = Me

M 552.9
Thermally- and air-stable chromium(0) compd. with four-membered chelate rings. Synth. by uv irradiation of $Cr(CO)_6$ with $MeN(PF_2)_2$ in Et_2O or by metal-vapour synth. Volatile, air-stable colourless solid. Sol. Et_2O, solns. slowly dec. Mp 182-183°. Bp 256°.

King, R.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1977, 142 (*synth, ir, P-31 nmr, pmr*)

King, R.B. *et al*, *Inorg. Chem.*, 1978, **17**, 2390; 1979, **18**, 364 (*synth, ir, nmr, ms*)
Chang, M. *et al*, *Inorg. Chim. Acta*, 1978, **30**, L341.

IC-003677

$C_3H_9CrO_3$

Chromium(*III*) methoxide
Trimethoxychromium(III). *Methyl chromate*(III). *Methanol, chromium*(3+) *salt* (*3:1*)

$Cr(OMe)_3$

M 145.0
Approx. octamer. Synth. from $(NH_4)_2CrO_4$ suspended in hot, dry MeOH in uv light; or from $CrCl_3(THF)_3$ and LiOMe in $MeOH/C_6H_6$. Grey-green powder. Insol. org. solvs., hydrol. by boiling H_2O. Mp >260°. μ_{eff} = $2.52\mu_B$ (294K). Antiferromagnetic.

Adams, R.W. *et al*, *Aust. J. Chem.*, 1966, **19**, 207.
Brown, D.A. *et al*, *J. Chem. Soc. A*, 1968, 1563 (*synth, uv, ir, raman*)
Mehrotra, R.C., *Adv. Inorg. Chem. Radiochem.*, 1983, **26**, 269 (*rev*)

IC-003678

$C_3H_9CrS_3$

Tris(methanethiolato)chromium(*III*), 9Cl
Tris(methylmercapto)chromium(III). *Chromium methylsulfide. Chromium methyl mercaptide*

$Cr(SMe)_3$

M 193.2
Layer struct. with Cr in octahedral CrS_6 sites. Green involatile solid with smell characteristic of parent disulfide. Insol. common org. solvs. μ_{eff} = $3.49\mu_B$ (298K), obeys Curie-Weiss law, θ 153K.

Brown, D.A. *et al*, *J. Chem. Soc. A*, 1969, 1510 (*synth, props, uv-vis, ir, struct, magnetism, raman*)

IC-003679

$C_3H_9Cu_2N_6S_3$

Triamminetris(thiocyanato)dicopper, 9Cl
Tri-μ-thiocyanatotriamminecopper(I)*copper*(II)
[12655-00-4]

$[Cu(NH_3)_3Cu(NCS)_3]_n$

M 352.4
Polymeric with $Cu^{I}(NCS)_4$ tetrahedra linked by bridging thiocyanate groups to *fac*-$Cu^{II}(NH_3)_3(SCN)_3$ octahedra, forming infinite sheets. Black needles.

[12151-69-8]

Garaj, J., *Chem. Zvesti*, 1965, **19**, 593 (*synth*)
Garaj, J., *Inorg. Chem.*, 1969, **8**, 304 (*cryst struct*)

IC-003680

$C_3H_9FeO_3$

Iron(*III*) methoxide
Ferric methoxide. Methanol iron(3+) *salt* (*3:1*)

$Fe(OMe)_3$

M 148.9
Trimeric struct. proposed. Synth. from $FeCl_3$ + MeOH + NH_3. Sol. C_6H_6. Magnetic props. support cluster formn.; antiferromagnetic coupling of $S = \frac{5}{2}$ Fe centres obsd.

Trimer:
$C_9H_{27}Fe_3O_9$ M 446.8

Bradley, D.C. *et al*, *J. Chem. Soc.*, 1958, 126 (*synth*)
Adams, R.W. *et al*, *Inorg. Chem.*, 1966, **5**, 346 (*magnetism*)

IC-003681

$C_3H_9FeO_9S_3$

Iron(*III*) methanesulfonate
Ferric methanesulfonate
[59640-42-5]

$Fe[OS(O)_2Me]_3$

M 341.1
Obt. from $MeSO_3Ag$ + $FeCl_3.6H_2O$. Light yellow solid.

Haynes, J.S. *et al*, *Can. J. Chem.*, 1981, **59**, 669 (*synth, mössbauer, ir, magnetism*)

IC-003682

$C_3H_9GaO_3$

Gallium(*III*) methoxide
Trimethoxygallium(III). *Methanol, gallium*(3+) *salt* (*3:1*)
[2746-72-7]

$Ga(OMe)_3$

M 162.8
Synth. from $Ga(OPr^i)_3$ + MeOH. White moisture-sensitive solid. Spar. sol. C_6H_6. $Subl._{0.4}$ 275-280°. Several other alkoxides also reported.

Bindal, S.R. *et al*, *J. Chem. Soc. A*, 1969, 863 (*synth, props, ir*)

IC-003683

$C_3H_9I_5PPt^{\ominus}$

Pentaiodo(trimethylphosphine)platinate(*IV*)(1−), 9Cl

$[PtI_5(PMe_3)]^{\ominus}$

M 905.6 (ion)
Tetrapropylammonium salt: [52309-25-8].
Black cryst. Sol. CH_2Cl_2, Me_2CO. Mp 145-150°.

Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 523 (*synth, ir, pmr*)

IC-003684

$C_3H_9LaO_3$

Lanthanum(*III*) methoxide
Trimethoxylanthanum(III)

$La(OMe)_3$

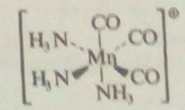
M 232.0
White powder. Sl. sol. MeOH. Presumably oligomeric.

Bradley, D.C. *et al*, *Chem. Ind.* (*London*), 1958, 1332.

IC-003685

$C_3H_9MnN_3O_3^{\oplus}$

Triamminetricarbonylmanganese(1+)
[14872-96-9]



M 190.0 (ion)

fac-form

Pentacarbonylmanganate(1−):
$C_8H_9Mn_3N_3O_8$ M 385.0
Synth. from $Mn_2(CO)_{10}$ and liq. NH_3. Air-stable yellow cryst. Sol. Me_2CO, H_2O.
Tetraphenylborate: [14872-95-8].
Yellow cryst. (Me_2CO aq.). Sol. Me_2CO, insol. H_2O.

Behrens, H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **349**, 241 (*synth*)
Behrens, H. *et al*, *J. Organomet. Chem.*, 1972, **34**, 367 (*synth*)
Herberhold, M. *et al*, *J. Organomet. Chem.*, 1978, **152**, 329 (*pmr, cmr, ir, cryst struct, props*)

IC-003686

$C_3H_9MnN_3O_6P$

Trinitrosyl(trimethyl phosphite-*P*)manganese, 9CI

[52352-74-6]

$Mn(NO)_3P(OMe)_3$

M 269.0

Synth. from $Mn(NO)_3(THF)$ and $P(OMe)_3$. Dark green cryst. Ir ν_{NO} 1788, 1690 cm^{-1} (THF).

Herberhold, M. *et al*, *J. Organomet. Chem.*, 1974, **67**, 81 (*synth, ir*)

IC-003687

$C_3H_9MoOS_3Si^{\ominus}$

Trimethylsiloxytrisulfidomolybdate(*VI*)(1−)

Trithioxo(trimethylsilanolato)molybdate(VI)(*1−*)

$[MoS_3(OSiMe_3)]^{\ominus}$

M 281.3 (ion)

Approx. tetrahedral at Mo.

Ph_4P salt: [96211-55-1].

Synth. by reaction of $[Mo_3O_7]^{2\ominus}$ with 7 equiv. of $(Me_3Si)_2S$ in MeCN. Red cryst. (Me_2CO/Et_2O at −20°). Sol. MeCN.

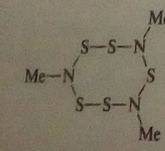
Do, Y. *et al*, *Inorg. Chem.*, 1985, **24**, 1831 (*cryst struct, synth, ir, uv-vis*)

IC-003688

$C_3H_9N_3S_5$

3,6,8-Trimethyl-1,2,4,5,7,3,6,8-pentathiatriazocine

[28924-10-9]



M 247.4

Isol. from reaction of $MeNH_2$ with SCl_2. White cryst; stable to NaOH aq. Sol. hexane. Bp 54-55°. Dec. at 190°.

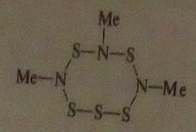
Stone, B.D. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 3580 (*synth, ir, raman, pmr*)

IC-003689

$C_3H_9N_3S_5$

4,6,8-Trimethyl-1,2,3,5,7,4,6,8-pentathiatriazocine

[28924-11-0]



M 247.4

White needles; stable to NaOH aq. Bp 44-46.5°.

Stone, B.D. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 3580 (*synth, ir, raman, pmr*)

IC-003690

$C_3H_9N_6NbO_3$

Diazidotrimethoxyniobium(*V*), 11CI

[97069-05-1]

$Nb(N_3)_2(OMe)_3$

M 270.0

Synth. from $Nb(OMe)_3Cl_2$ and KN_3. Moisture-sensitive solid. Insol. common org. solvs. Ir ν_{N_3} 2100 cm^{-1}. Dec. at 180°/0.4 mm.

▷ Potentially explosive.

Geetha, C.N. *et al*, *Indian J. Chem., Sect. A*, 1985, **24**, 236 (*synth, ir*)

IC-003691

$C_3H_9N_6NiS_3^{\ominus}$

Triamminetris(thiocyanato-*N*)nickelate(*II*)(1−)

$[Ni(NCS)_3(NH_3)_3]^{\ominus}$

M 284.0 (ion)

mer-Octahedral anion.

NH_4 salt: Deliquescent blue-violet trigonal cryst. μ_{eff} = 3.26μ_B.

Porai-Koshits, M.A. *et al*, *Acta Crystallogr.*, 1957, **10**, 784 (*cryst struct*)

Yukhno, E.R., *Zh. Neorg. Khim.*, 1960, **7**, 807; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 417 (*synth, magnetism*)

IC-003692

$C_3H_9N_6O_6Zn^{\ominus}$

Tris(carbazato)zincate(1−)

Tris(hydrazinecarboxylato-N^2,*O′)zincate(1−)*

$[(H_2NNHCO_2)_3Zn]^{\ominus}$

M 290.5 (ion)

6-Coordinate zinc; struct. not detd.

K salt: [14874-65-8].

Hydrazinium salt: [12076-76-5].

Forms a monohydrate.

[19697-27-9]

Braibanti, A. *et al*, *Ric. Sci.*, 1966, **36**, 1153, 1156 (*synth, ir*)
Slivnik, J. *et al*, *Monatsh. Chem.*, 1967, **98**, 200 (*synth*)
Braibanti, A. *et al*, *Inorg. Chem.*, 1968, **7**, 1430 (*ir, synth*)
Patil, K.C., *Synth. React. Inorg. Metal-Org. Chem.*, 1983, **13**, 29 (*synth, ir, thermal anal*)

IC-003693

C_3H_9O

Trimethyloxonium, 9CI, 8CI

$Me_3O^{\oplus}$

M 61.1

Powerful alkylating agent.

Tetrafluoroborate: [420-37-1]. *Trimethyloxonium tetrafluoroborate, 9CI, 8CI*

Methylating agent. Used as a derivatisation reagent in anal. of haemins. Commercially available. Colourless cryst. (CH_2Cl_2). Sol. CH_2Cl_2. Mp 141-143° dec.

2,4,6-Trinitrobenzenesulfonate: Powerful alkylating agent. Cryst. (EtOAc/Me_2CO). Mp 115-120° dec. (remelts at 181-183°).

Pettit, D.J. *et al*, *J. Org. Chem.*, 1963, **28**, 2932.
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 435; **6**, 630.
Org. Synth., Coll. Vol., 5, 1973, 1099.
Dean, R.T. *et al*, *Anal. Biochem.*, 1976, **76**, 1 (*use*)

IC-003694

$C_3H_9O_3P$

Trimethyl phosphite, 9CI, 8CI

Trimethoxyphosphine. Trimethoxyphosphorus(III). *Trimethoxophosphorus*(III)

[121-45-9]

$P(OMe)_3$

M 124.0

Reagent for dehydrohalogenations, debrominations and deoxygenations, used in Corey-Winter synth. Uses similar to those of Triethyl phosphite, IC-005239. Air-sensitive liq. with powerful sickly odour. d_4^{20} 1.052. Mp −78°. Bp 111-112°, Bp_{23} 22°. n_D^{20} 1.4080. Forms complexes with cuprous halides.

▷ TLV 2-6. Flammable. Powerful obnoxious odour. Induces headache. TH1400000.

Meyrick, C.I. *et al*, *J. Chem. Soc.*, 1950, 225 (*ir, raman*)
Halman, M. *et al*, *J. Chem. Soc.*, 1963, 2853 (*uv*)
Goodell, L.J. *et al*, *Can. J. Chem.*, 1969, **47**, 2461 (*pmr*)
Verstuyft, A.N. *et al*, *Inorg. Chem.*, 1976, **15**, 732 (*cmr*)
Cowley, A.H. *et al*, *Inorg. Chem.*, 1977, **16**, 854; 1984, **23**, 3378 (*pe*)
Griend, L.J.V. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 2459 (*props, struct*)
Gray, G.A. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 3243 (*nmr*)
Labintsev, V.B. *et al*, *Zh. Org. Khim.*, 1977, **13**, 1141; *J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 1050 (*ms*)
Organophosphorus Reagents in Org. Synth., (J.I.G. Cadogan, Ed.), Academic Press, 1979 (*uses*)
Chattopadhyay, S. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1981, **24**, 27 (*pe*)
Vasil'ev, V.V. *et al*, *Zh. Obshch. Khim.*, 1981, **51**, 2134; *J. Gen. Chem. USSR (Engl. Transl.)*, 1981, **51**, 1836 (*O-17 nmr*)
Worley, S.D. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1982, **25**, 135 (*struct*)
Sodhi, R.N. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1983, **32**, 283 (*struct, pe*)
Cload, P.A. *et al*, *Org. Mass Spectrom.*, 1983, **18**, 57 (*ms*)
Bart, J.C.J. *et al*, *Phosphorus Sulfur*, 1983, **17**, 205 (*conformn, complexes*)
Holtzclaw, J.R. *et al*, *Org. Mass Spectrom.*, 1985, **20**, 90 (*ms, struct*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 452.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 524.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3398.

IC-003695

$C_3H_9O_4P$

Trimethyl phosphate, 9CI

Trimethoxooxophosphorus(V)

[512-56-1]

$(MeO)_3P{=}O$

M 140.0

Solvent for aromatic halogenations and nitrations. Methylating agent for nitrogen heterocyclic compds. Pleasant smelling liq. Sol. H_2O, org. solvs. d_4^{20} 1.21. Bp 196°, Bp_{50} 110°, Bp_5 62°. n_D^{20} 1.3963.

▷ Shows delayed toxicity. TC8225000.

Evans, D.P. *et al*, *J. Chem. Soc.*, 1930, 1310 (*synth*)
Yamauchi, K. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1973, 391 (*props, use*)
Pearson, D.E. *et al*, *Synthesis*, 1976, 621 (*use*)
Cowley, A.H. *et al*, *Inorg. Chim. Acta*, 1977, **25**, L151 (*pe*)
Burkhardt, W.D. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **442**, 19 (*ir, raman*)
Lowe, G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1979, 733 (*O-17, P-31 nmr*)
Wolff, R. *et al*, *Z. Phys. Chem. (Leipzig)*, 1980, **261**, 726 (*struct*)
Kawazoe, Y. *et al*, *Chem. Pharm. Bull.*, 1982, **30**, 2077 (*props, use*)
Cload, P.A. *et al*, *Org. Mass Spectrom.*, 1983, **18**, 57 (*ms*)
Cowley, A.H. *et al*, *Inorg. Chem.*, 1984, **23**, 3378 (*pe*)
Cohen, J.S. *et al*, *J. Magn. Reson.*, 1984, **59**, 181 (*pmr*)
Appling, J.R. *et al*, *Org. Mass Spectrom.*, 1985, **20**, 343 (*ms*)
Yarkov, A.V. *et al*, *Zh. Obshch. Khim.*, 1985, **55**, 50; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 42 (*ir, raman, conformn*)
Taga, K. *et al*, *J. Mol. Struct.*, 1989, **212**, 157 (*raman, struct*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3397.
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 402.

IC-003696

$C_3H_9O_4ReSi$

Trioxo(trimethylsilanolato)rhenium(*VII*)

Trimethylsilyl perrhenate. Perrhenic acid trimethylsilyl ester, 9CI

[16687-12-0]

$Me_3SiOReO_3$

M 323.3

Synth. from Re_2O_7 and $(Me_3Si)_2O$ or from $AgReO_4$ and Me_3SiCl. Colourless cryst. (hot $(Me_3Si)_2O$ or by subl.), sensitive to hydrolysis. Insol. hydrocarbons. Mp 79.5-80.5°. $Subl._{0.1}$ 65-80°.

Schmidt, M. *et al*, *Chem. Ber.*, 1959, **92**, 2667 (*synth, props*)
Inorg. Synth., 1967, **9**, 149 (*synth, props*)
Sheldrick, G.M. *et al*, *J. Chem. Soc. A*, 1969, 2160 (*cryst struct*)
Schmidbaur, H. *et al*, *Chem. Ber.*, 1974, **107**, 2697 (*nqr*)

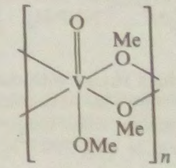
IC-003697

$C_3H_9O_4V$

Trimethoxy(oxo)vanadium(*V*), 11CI

Methyl vanadate. Oxotrimethoxyvanadium(V). *Vanadic acid trimethyl ester, 9CI*

[7681-91-6]



M 160.0

Struct. comprises chains of distorted octahedra. All V=O on same side of the chain. Synth. from $VOCl_3$ + NaOMe in MeOH or from V_2O_5, MeOH and trimethylorthoformate or by MeO exchange with other alkoxides. Used in olefin polym. catalysts and in vapour phase epitaxy to form gallium arsenide field effect transisitors. Yellow solid.

Caughlan, C.N. *et al*, *Inorg. Chem.*, 1966, **5**, 2131 (*synth from $VOCl_3$, cryst struct*)
Ger. Pat., 2 343 056, (1975); *CA*, **83**, 113667e (*synth from V_2O_5*)
Adler, B. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **431**, 227 (*ms*)
Japan. Pat., 59 169 123, (1984); *CA*, **102**, 124032f (*use*)
U.S. Pat., 4 525 468, (1985); *CA*, **104**, 51248h (*use, polym*)

IC-003698

$C_3H_9O_9S_3Sb$

Tris(methanesulfonato-*O*,*O′*)antimony

[110899-39-3]

$Sb(O_3SMe)_3$

M 407.0

V. moisture-sensitive solid. Sol. MeOH, DMF and DMSO forming ionising solns., insol. $PhNO_2$, $MeNO_2$, MeCN. Begins to dec. at 45-50°.

Kapoor, R. *et al*, *Can. J. Chem.*, 1987, **65**, 1195 (*synth, props, reactions*)

IC-003699

$C_3H_{10}AgN_7S_3$

Bis(hydrazinecarbothioamide-*S*)(thiocyanato-*N*)silver(*I*), 12Cl

[108089-46-9]

$[H_2NNHC(NH_2)=S]_2AgNCS$

M 348.2

Cryst.

Nardelli, M. *et al*, *Ric. Sci.*, 1965, **35**, 480 (*synth*)
Calzolari, C.L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 910 (*struct*)
Bonamartini, A.C. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 407 (*struct*)

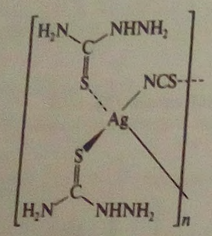
IC-003700

$C_3H_{10}AgN_7S_3$

***catena*-μ-(Thiocyanato)bis(thiosemicarbazide)silver(*I*)**

Bis(thiosemicarbazide)silver(I) *thiocyanate*

[29381-05-3]



M 348.2

Polymeric double chain struct. with distorted trigonal pyramidal silver. May also be considered to be pentagonal bipyramidal when longer contacts are taken into account. Cryst. Ir $\nu_{C\equiv N}$ 2083; ν_{C-S} 790 cm^{-1}.

Capacchi, L.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 910 (*cryst struct, ir*)

IC-003701

$C_3H_{10}BF_2N$

Difluorohydro(trimethylamine)boron

(*N,N-Dimethylmethanamine*)*difluorohydroboron*, *10Cl*. *N,N-Dimethylmethanamine compd. with difluoroborane* (*1:1*), *9Cl*. *Difluoroborane trimethylamine*

[35237-72-0]

$Me_3N{-}BHF_2$

M 108.9

White solid. Mp 124-125°.

Van Paasschen, J.M. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2680 (*synth, ir, nmr, pmr*)
Mogeot, H. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 825 (*ir, raman*)
Tuchagues, J.-P. *et al*, *J. Organomet. Chem.*, 1973, **54**, 69 (*ir, nmr*)
Geanangel, R.A., *Inorg. Chem.*, 1975, **14**, 696 (*nmr*)
Van Paasschen, J.M. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 2321.
Van Paasschen, J.M. *et al*, *Inorg. Chem.*, 1978, **17**, 3302.

IC-003702

$C_3H_{10}BO_3^{\ominus}$

Hydrotrimethoxyborate(1−), 10Cl, 9Cl, 8Cl

Trimethoxyhydroborate. Trimethoxyborohydride

[54787-85-8]

$[(MeO)_3BH]^{\ominus}$

M 104.9 (ion)

Li salt: [39659-89-7].
$C_3H_{10}BLiO_3$ M 111.8
No phys. props. reported.

Na salt: [16940-17-3].
$C_3H_{10}BNaO_3$ M 127.9
Intermed. in methanolysis of $NaBH_4$. Selective reducing agent. Catalyst for manuf. of foamed polyamides. Used as sterilant for control of screwworm flies. Solid, stable in dry air. Sol. dioxan, isopropylamine, NH_3. Mp *ca.* 230° dec. Reacts with H_2O, alcohols.

▷ Flammable.

K salt: [63637-24-1].
$C_3H_{10}BKO_3$ M 144.0
No phys. props. reported.

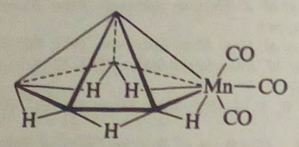
Brown, H.C. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 192 (*synth*)
Japan. Pat., 62 10 567, (1962); *CA*, **58**, 11545a (*use*)
Mikheeva, V.I. *et al*, *Zh. Neorg. Khim.*, 1967, **12**, 2019; *CA*, **67**, 121875f (*synth*)
Japan. Pat., 72 39 297, (1972); *CA*, **78**, 137304g (*use*)
Kadlec, V. *et al*, *Collect. Czech. Chem. Commun.*, 1974, **39**, 3200 (*synth*)
Mindl, J. *et al*, *Collect. Czech. Chem. Commun.*, 1976, **41**, 3314 (*use, props*)
Niehues, K.J., *CA*, 1980, **93**, 196748n (*rev*)

IC-003703

$C_3H_{10}B_5MnO_3$

Tricarbonyl[decahydropentaborato(2−)]manganese, 11Cl

[71230-48-3]



M 203.1

Proposed struct. shown. Yellow liq. Insol. H_2O. Mp −2.5° to −2.3°. Ir ν_{CO} 2065s, 1970vs, 1900vw cm^{-1} (liq. film). May be deprotonated to give Tricarbonyl[nonahydropentaborato(2−)] manganate(1−), IC-003665.

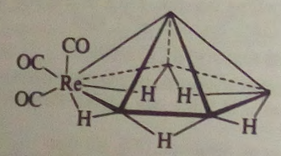
Fischer, M.B. *et al*, *Inorg. Chem.*, 1979, **18**, 3200 (*synth, ir, B-11 nmr, pmr*)
Organomet. Synth., 1988, **4**, 125 (*synth, ir, pmr, B-11 nmr, uv, ms, reactions*)

IC-003704

$C_3H_{10}B_5O_3Re$

Tricarbonyl[(1,2,5-η)-decahydropentaborato(1−)-H^2,H^5]rhenium, 11Cl

[98586-75-5]



M 334.3

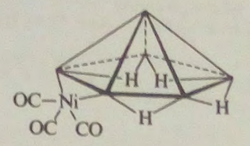
Proposed struct. shown. Solid. Sol. C_6H_6.

Coons, D.E. *et al*, *Inorg. Chem.*, 1985, **24**, 3774 (*synth, pmr, B-11 nmr, ms*)

IC-003705

$C_3H_{10}B_6NiO_3$

Tricarbonyl[η³-hexaborane(10)]nickel



M 217.6

Seems to be in equilibrium with starting materials and is consistent with formation of weakly bound $Ni(CO)_3$ complex. Impure yellow liq.

Davidson, A. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 2802 (*synth*)

IC-003706

$C_3H_{10}Cl_2CrN_2$

Dichloro(1,3-propanediamine)chromium(*II*), 8Cl

Dichloro(*1,3-diaminopropane*)*chromium*(II)

[33826-33-4]

$[CrCl_2(H_2NCH_2CH_2CH_2NH_2)]_n$

M 197.0

6-Coordinate chloride bridged polymer. Light blue air-sensitive solid. μ_{eff} = 3.87μ_B (300K); 2.14μ_B (90K).

Larkworthy, L.F. *et al*, *J. Chem. Soc. A*, 1971, 2766 (*synth, props*)

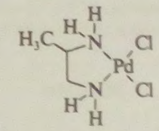
IC-003707

$C_3H_{10}Cl_2N_2Pd$

Dichloro(1,2-propanediamine-*N,N'*)palladium, 9Cl

Dichloro(*1,2-diaminopropane*)*palladium*(II)

[27952-37-0]



M 251.4

No phys. props. reported.

[17653-67-7, 90941-07-4]

Durig, J.R. *et al*, *Spectrochim. Acta*, 1965, **21**, 1367 (*ir*)
Ito, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 2584 (*uv, cd*)
Nakayama, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1984, **57**, 1336 (*uv, cd, mcd*)

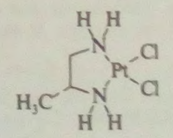
IC-003708

$C_3H_{10}Cl_2N_2Pt$

Dichloro(1,2-propanediamine-*N,N'*)platinum, 9Cl

Dichloro(*1,2-diaminopropane*)*platinum*(II), *8Cl*

[33727-98-9]



(*R*)-*form*

M 340.1

Chiral complex. Potential antitumour agent. Yellow solid. Sol. 0.5M HCl.

▷ TP2497350.

(***R*)-*form*** [17668-31-4]

(***S*)-*form*** [56298-00-1]

More mutagenically active than (*R*)-form.

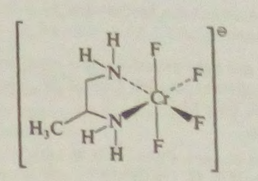
Beattie, J.K. *et al*, *Inorg. Chem.*, 1975, **14**, 996 (*synth*)

Nakayama, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1984, **57**, 1336 (*uv-vis, cd, mcd*)
Fanizzi, F.P. *et al*, *Inorg. Chim. Acta*, 1987, **137**, 45 (*pharmacol*)

IC-003709

$C_3H_{10}CrF_4N_2^{\ominus}$

Tetrafluoro(1,2-propanediamine-*N,N'*)chromate(*III*)(1−), 11Cl, 9Cl



M 202.1 (ion)

Struct. by analogy with (Ethylenediamine) tetrafluorochromate(*III*)(1−), IC-003290.

Na salt: [40961-77-1].
Pale blue solid + H_2O + 1.15$NaClO_4$.

Difluorobis(*1,2-propanediamine*-N,N')*chromium*(III) *salt:* see *Difluorobis*(*1,2-propanediamine*-N,N')*chromium*(III)(*1+*), *IC-005446*

H deriv., compd. with 1,2-propanediamine hydrochloride (*1:1:1*): [95786-54-2].
Blue solid.

Vaughn, J.W. *et al*, *Inorg. Chem.*, 1973, **12**, 2346 (*synth*)
Díaz, C. *et al*, *Transition Met. Chem.*, 1984, **9**, 469 (*synth, ir, uv-vis*)

IC-003710

$C_3H_{11}BBrP$

Bromodihydro(trimethylphosphine)boron, 10Cl

Bromoborane trimethylphosphine. Trimethylphosphine compd. with bromoborane, *9Cl*

[60228-69-5]

$Me_3P{-}BH_2Br$

M 168.8

Mp 61.0-62.5°. Erroneous coupling constants have been reported for this compd.

Dennison, M.L. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 979 (*nmr, synth*)
Jugie, G. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 900 (*nmr*)
Sisler, H.H. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1745 (*ir, pmr*)
Schmidbaur, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1981, **20**, 283.

IC-003711

$C_3H_{11}BClP$

Chlorodihydro(trimethylphosphine)boron, 10Cl

Chloroborane trimethylphosphine. Trimethylphosphine, compd. with chloroborane(*1:1*)

[64160-46-9]

$Me_3P{-}BH_2Cl$

M 124.3

Cryst. (Et_2O/pentane). Mp 73°.

Jugie, G. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 900.
Sisler, H.H. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1745 (*synth, ir, pmr*)
Kodama, G. *et al*, *Inorg. Chem.*, 1979, **18**, 3302 (*synth*)
Kameda, M. *et al*, *Inorg. Chem.*, 1980, **19**, 2288 (*synth, nmr*)
Schmidbaur, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1981, **20**, 283 (*synth, ir, nmr*)

$C_3H_{11}BIN$ IC-003712

Dihydroiodo(trimethylamine)boron

(N,N-Dimethylmethanamine)dihydroiodoboron, 10CI. N,N-Dimethylmethanamine compd. with iodoborane (1:1), 9CI. Iodoborane compd. with trimethylamine (1:1), 8CI

[25741-81-5]

$Me_3N{-}BH_2I$

M 198.8

Moisture- and light-sensitive white cryst. solid (CCl_4/cyclohexane). Sol. CCl_4, C_6H_6, insol. alkanes. Mp 73°. Subl. near Mp.

▷ YH2720000.

Lowe, J.R. *et al, Inorg. Chem.*, 1970, **9**, 1423.
Inorg. Synth., 1970, **12**, 116 (*synth*)
Brown, M.P. *et al, J. Chem. Soc. A*, 1970, 410 (*ir*)
Bratt, P.J. *et al, Inorg. Chim. Acta*, 1974, **10**, 191 (*ir*)
Myers, W.H. *et al, Inorg. Chem.*, 1975, **14**, 2874 (*pmr*)
Denniston, M.L. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 379 (*pmr, nmr*)

$C_3H_{11}BIP$ IC-003713

Dihydroiodo(trimethylphosphine)boron, 10CI

Iodoborane trimethylphosphine. Iodoborane complex with trimethylphospine, 9CI. Trimethylphosphine iodoborane

[60228-73-1]

$Me_3P{-}BH_2I$

M 215.8

Moisture-sensitive cryst. (CH_2Cl_2/pet. ether). Mp 69.5-71°.

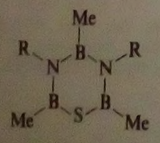
Denniston, M.L. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 979 (*synth*)
Sisler, H.H. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 1745 (*synth, nmr, ir*)
Pennington, B.T. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 389 (*synth, pmr*)

$C_3H_{11}B_3N_2S$ IC-003714

2,4,6-Trimethyl-1,3,5,2,4,6-thiadiazatriborinane

Tetrahydro-2,4,6-trimethyl-1,3,5,2,4,6-thiadiazatriborine, 10CI

[63261-95-0]



R = H

M 139.6

Liq., air- and moisture-sensitive. Sol. Et_2O.

Nölle, D. *et al, Chem. Ber.*, 1977, **110**, 1643 (*B-11 nmr, N-14 nmr*)

$C_3H_{12}AlN$ IC-003715

Trihydro(trimethylamine)aluminium

Aluminium hydride trimethylamine. Trimethylamine-alane. (N,N-Dimethylmethanamine)trihydroaluminium, 9CI

[16842-00-5]

$Me_3N{\cdot}AlH_3$

M 89.1

Synth. from $LiAlH_4$ + $[Me_3NH]Cl$. White, v. air- and moisture-sensitive solid. Mp 76°.

Ruff, J.K. *et al, J. Am. Chem. Soc.*, 1960, **82**, 2141 (*synth*)
Fraser, G.W. *et al, J. Chem. Soc.*, 1963, 3742 (*synth, ir, raman*)
Roszinski, H. *et al, Z. Phys. Chem. (Munich)*, 1963, **36**, 26 (*ir*)
Sawodny, W. *et al, Z. Phys. Chem. Neue Folge*, 1965, **44**, 227 (*ir, raman*)
Inorg. Synth., 1967, **9**, 30 (*synth*)
Semenenko, K.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 949 (*ir*)
Almenningen, A. *et al, Acta Chem. Scand.*, 1972, **26**, 3928 (*ed*)
Semenenko, K.N. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 1921 (*dipole moment*)

$C_3H_{12}BN$ IC-003716

Trihydro(trimethylamine)boron

Borane trimethylamine. (N,N-Dimethylmethanamine) trihydroboron, 10CI. N,N-Dimethylmethanamine, compd. with borane(1:1). Trimethylamine borane

[75-22-9]

$Me_3N{-}BH_3$

M 72.9

Commercially available. Source of borane for the reduction of ketones and Schiff bases and for hydroboration of alkenes. White cryst. solid. Stable, easy to handle. Insol. hexane, v. sol. most org. solvs., sl. sol. H_2O, cyclohexane.

▷ PA0525000.

Burg, A.B. *et al, J. Am. Chem. Soc.*, 1937, **59**, 780 (*synth*)
Billman, J.H. *et al, J. Org. Chem.*, 1962, **27**, 2640 (*use*)
Larsen, L.A. *et al, Inorg. Chem.*, 1974, **13**, 2284 (*ms*)
Beachley, O.T. *et al, Inorg. Chem.*, 1975, **14**, 120 (*ir, pmr*)
Cassoux, P. *et al, Inorg. Chem.*, 1975, **14**, 126 (*far ir*)
Geanangel, R.A., *Inorg. Chem.*, 1975, **14**, 696 (*nmr, cmr*)

$C_3H_{12}BN_3$ IC-003717

Tris(methylamino)borane, 8CI

N,N′,N″-Trimethylboranetriamine, 10CI, 9CI

[7397-44-6]

$B(NHMe)_3$

M 100.9

Liq., sensitive to moisture. Sol. nonpolar solvs. d_4^{20} 0.887. Bp_{48} 70-80°. n_D^{25} 1.4432.

Aubrey, D.W. *et al, J. Chem. Soc.*, 1959, 2927 (*synth, props*)
English, W.D. *et al, J. Am. Chem. Soc.*, 1961, **83**, 2122 (*synth*)
Davis, F.A. *et al, J. Org. Chem.*, 1971, **36**, 1300 (*nmr*)
Beck, W. *et al, Chem. Ber.*, 1972, **105**, 2883 (*nmr*)
Niedenzu, K. *et al, Z. Anorg. Allg. Chem.*, 1972, **387**, 107 (*nmr*)
Beachley, O.T. *et al, Inorg. Chem.*, 1977, **16**, 2935 (*pmr, props*)
Almenningen, A. *et al, Acta Chem. Scand., Ser. A*, 1981, **35**, 341 (*struct*)

$C_3H_{12}BO_3P$ IC-003718

Trihydro(trimethyl phosphite-*P*)boron, 10CI

Borane trimethyl phosphite. Phosphorous acid trimethyl ester compd. with borane (1:1), 9CI, 8CI. Methyl phosphite compd. with borane

[6867-39-6]

$(MeO)_3P{-}BH_3$

M 137.9

Liq. Bp_{23} 86°. n_D^{25} 1.4162.

Reetz, T., *J. Am. Chem. Soc.*, 1960, **82**, 5039 (*synth*)
McFarlane, H.C.E. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 1300 (*nmr*)
Fussstetter, H. *et al, Chem. Ber.*, 1977, **110**, 3172 (*nmr*)
Griend, V. *et al, J. Am. Chem. Soc.*, 1977, **99**, 2459 (*ir, nmr*)
Hassler, K., *Ber. Bunsenges. Phys. Chem.*, 1980, **84**, 285 (*ir, raman*)
Cowley, A.H. *et al, Inorg. Chem.*, 1982, **21**, 85 (*pe*)

$C_3H_{12}BP$ IC-003719

Trihydro(trimethylphosphine)boron, 10CI

Borane trimethylphosphine. Trimethylphosphine compd. with borane (1:1), 8CI. Trimethylphosphine borine

[1898-77-7]

$Me_3P{-}BH_3$

M 89.9

Solid. Antiknock agent in petrol. Mp 103-103.5°.

Burg, A.B. *et al, J. Am. Chem. Soc.*, 1953, **75**, 3872.
Sisler, H.H. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 1745 (*ir*)
Van Paasschen, J.M. *et al, Inorg. Chem.*, 1978, **17**, 3302.
Apel, J. *et al, Z. Anorg. Allg. Chem.*, 1979, **453**, 28 (*nmr*)
Cowley, A.H. *et al, Inorg. Chem.*, 1982, **21**, 85 (*pe*)
Kameda, M. *et al, Inorg. Chem.*, 1982, **21**, 1267 (*nmr*)

$C_3H_{12}B_3N_3$ IC-003720

2,4,6-Trimethylborazine, 10CI, 9CI, 8CI

B,B,B-Trimethylborazole

[5314-85-2]

As Borazine, IC-001044 with

R = Me, R′ = H

M 122.5

Solid with unpleasant odour. Sol. most org. solvs.; v. slowly hydrol. by H_2O. Mp 29-31°. Bp 129°, Bp_{20} 35°. V.p. 16.3 mm at 29.8°. Trouton constant 23.3 e.u. High thermal stability.

Schlesinger, H.I. *et al, J. Am. Chem. Soc.*, 1936, **58**, 409 (*synth*)
Haworth, D.T. *et al, J. Am. Chem. Soc.*, 1960, **82**, 3860 (*ir, synth*)
Wagner, R.I. *et al, Inorg. Chem.*, 1962, **1**, 93 (*ir, synth*)
Anzenhofer, K., *Mol. Phys.*, 1966, **11**, 495 (*cryst struct*)
Nöth, H. *et al, J. Organomet. Chem.*, 1968, **12**, 23 (*pmr*)
Wrackmeyer, B. *et al, Chem. Ber.*, 1976, **109**, 3480 (*nmr*)
Blick, K.E. *et al, Z. Anorg. Allg. Chem.*, 1978, **442**, 183 (*ir*)
Nöth, H. *et al, Chem. Ber.*, 1981, **114**, 1150 (*nmr*)

$C_3H_{12}Cl_3CrN_6S_3$ IC-003721

Trichlorotris(thiourea-*S*)chromium(*III*), 10CI, 9CI

Chromium(III) chloride tris(thiourea)

[15189-61-4]

$CrCl_3[S{=}C(NH_2)_2]_3$

M 386.7

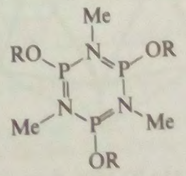
Stereochem. not reported. Dark red solid. Insol. Me_2CO, sol. MeOH. Mp 225°, Mp 245°. Dec. begins at 220°. One thiourea molecule is lost at 222-275°, then another at ~380°; the last is lost at temps. up to 480°.

Klan, M.M. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 1621 (*reactions, props, ir*)
Janicki, H. *et al, J. Therm. Anal.*, 1976, **9**, 401 (*thermal dec*)

$C_3H_{12}N_3O_3P_3$ IC-003722

1,2,3,4,5,6-Hexahydro-2,4,6-trihydroxy-1,3,5-trimethyl-1,3,5,2,4,6-triazatriphosphorine, 11CI

2,4,6-Trihydroxy-1,3,5-trimethylcyclotriazaphosphane



R = H

M 231.0

Each ester consists of a mixt. of (2*a*,4*a*,6*a*) and (2*a*,4*a*,6*β*) stereoisomers.

O,O′,O″-*Trimethyl*: *1,2,3,4,5,6-Hexahydro-2,4,6-trimethoxy-1,3,5-trimethyl-1,3,5,2,4,6-triazatriphosphorine*
$C_6H_{18}N_3O_3P_3$ M 273.1
Colourless liq. $Bp_{0.3}$ 58-60°.

O,O′,O″-*Triethyl*: [77834-36-7]. *2,4,6-Triethoxy-1,2,3,4,5,6-hexahydro-1,3,5-trimethyl-1,3,5,2,4,6-triazatriphosphorine*
$C_9H_{24}N_3O_3P_3$ M 315.2
Colourless liq. $Bp_{0.3}$ 86°.

O,O′,O″-*Triisopropyl*: [77834-37-8]. *1,2,3,4,5,6-Hexahydro-2,4,6-triisopropoxy-1,3,5-trimethyl-1,3,5,2,4,6-triazatriphosphorine*
$C_{12}H_{30}N_3O_3P_3$ M 357.3
Colourless oil. $Bp_{0.5}$ 105-107°.

O,O′,O″-*Tri-tert-butyl*: [77834-38-9]. *2,4,6-Tri-tert-butoxy-1,2,3,4,5,6-hexahydro-1,3,5-trimethyl-1,3,5,2,4,6-triazatriphosphorine*
$C_{15}H_{36}N_3O_3P_3$ M 399.3
Colourless oil. $Bp_{0.15}$ 110°.

O,O′,O″-*Triphenyl*: [77834-39-0]. *1,2,3,4,5,6-Hexahydro-1,3,5-trimethyl-2,4,6-triphenoxy-1,3,5,2,4,6-triazatriphosphorine*
$C_{21}H_{24}N_3O_3P_3$ M 459.3
Non-distillable, pale yellow oil.

[77834-36-7, 77834-37-8, 77834-38-9, 77834-39-0, 77881-22-2, 77881-23-3, 77881-24-4, 77881-25-5, 81798-56-3, 81845-18-3]

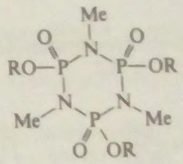
Zeiss, W. *et al, Z. Anorg. Allg. Chem.*, 1981, **475**, 256 (*synth, pmr, cmr, P-31 nmr*)

$C_3H_{12}N_3O_6P_3$ IC-003723

1,2,3,4,5,6-Hexahydro-2,4,6-trihydroxy-1,3,5-trimethyl-1,3,5,2,4,6-triazatriphosphorine 2,4,6-trioxide

1,3,5-Trimethyl-2,4,6-trihydroxycyclotriazaphosphane 2,4,6-oxide

[84227-55-4]



R = H

M 279.0

O,O′,O″-*Trimethyl*: [1085-76-3]. *2,4,6-Trimethoxy-1,3,5-trimethyl-1,2,3,4,5,6-hexahydro-1,3,5,2,4,6-thiazatriphosphorine 2,4,6-trioxide*
$C_6H_{18}N_3O_6P_3$ M 321.1
Colourless cryst. (CH_2Cl_2/pet. ether). Mp 128°. $Subl_{0.1}$ 120°.

[75801-79-5]

Fitzsimmons, B.W. *et al, J. Chem. Soc.*, 1964, 4459; 1965, 7432 (*synth*)
Branton, G.R. *et al, J. Chem. Soc. A*, 1970, 151 (*pe*)
Ferrar, W.T. *et al, Macromolecules*, 1980, **13**, 1345 (*props, pmr, cmr, P-31 nmr*)
Dhathathreyan, K.S. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1928 (*synth, pmr, cmr, P-31 nmr*)
Thomas, B. *et al, Z. Anorg. Allg. Chem.*, 1982, **490**, 121 (*ir, N-15 nmr, P-31 nmr*)

IC-003724

$C_3H_{12}N_6O_3S_5Zn$

[(Monothiosulfato(2−)-*S*)]tris(thiourea-*S*)zinc

Tris(thiourea)zinc thiosulfate

[19596-75-9]

$Zn(SSO_3)[S{=}C(NH_2)_2]_3$

M 405.8

Tetrahedral at Zn. Cryst. + $1H_2O$ (H_2O).

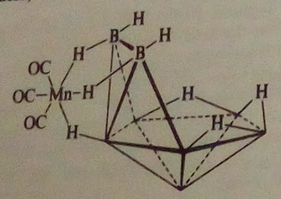
[19596-74-8]

Nardelli, M. *et al*, *Gazz. Chim. Ital.*, 1958, **88**, 832 (*synth*)
Flint, C.D. *et al*, *J. Chem. Soc. A*, 1967, 1718 (*synth, ir*)
Andreeti, G.D. *et al*, *Ric. Sci.*, 1968, **38**, 1110 (*cryst struct*)
Freedman, A.N. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 1455 (*ir*)
Gabelica, Z., *Bull. Soc. Chim. Belg.*, 1977, **86**, 851 (*ir*)

IC-003725

$C_3H_{13}B_8MnO_3$

Tricarbonyl[tridecahydrooctaborato(1−)-H^1,H^2,H^6]manganese, 9CI



M 238.5

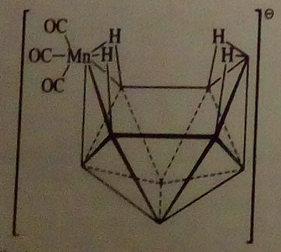
nido-. Golden yellow air-sensitive cryst. (by chromatog. then subl.). Sol. CH_2Cl_2. Mp 66-67°. Subl. 45-52° *in vacuo*. Ir ν_{CO} 2090vs, 1955vs cm^{-1} (KBr).

Gaines, D.F. *et al*, *Inorg. Chem.*, 1974, **13**, 2261 (*synth, deriv*)
Calabrese, J.C. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 6318 (*cryst struct, raman, synth, ir, ms, uv, B-11 nmr, pmr, props*)

IC-003726

$C_3H_{13}B_9MnO_3^{\ominus}$

Tricarbonyl[(6,7,8-η)-tridecahydrononaborato(2−)-H^6,H^8]manganate(1−), 9CI



M 249.3 (ion)

Me_4N salt: [41729-34-4].

Air-stable reddish/orange cryst. (CH_2Cl_2/heptane). Possesses high thermal, hydrolytic and oxidative stability. Sol. CH_2Cl_2, THF, MeCN. Mp 200° dec. Ir ν_{CO} 2060s, 2025vs, 2005vs cm^{-1}.

Lott, J.W. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 3042 (*synth, ir, pmr, B-11 nmr, uv-vis*)
Lott, J.W. *et al*, *Inorg. Chem.*, 1974, **13**, 2261 (*uv, ir, pmr, B-11 nmr*)
Organomet. Synth., 1988, **4**, 130 (*synth, ir, B-11 nmr*)

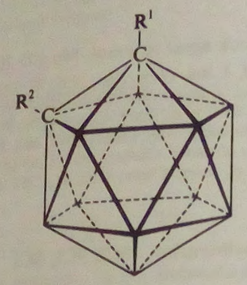
IC-003727

$C_3H_{13}B_{10}ClHg$

Chloro(2-methyl-1,2-dicarbadodecaboran(12)-1-yl)mercury, 9CI, 8CI

Chloro(methyl-o-carboranyl)mercury. (Methyl-o-carboranyl)chloromercury. Methylbarenylmercury chloride

[26469-52-3]



R^1 = HgCl, R^2 = Me

M 393.2

Cryst. (toluene). Mp 272-273°.

Zakharkin, L.I. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 667 (*synth, deriv*)
Denisovich, L.I. *et al*, *J. Organomet. Chem.*, 1973, **57**, 87 (*electrochem*)

IC-003728

$C_3H_{13}B_{10}ClHg$

Chloro(7-methyl-1,7-dicarbadodecaboran(12)-1-yl)mercury

1-Chloromercuri-7-methyl-m-*carborane. [7-Methyl-1,7-dicarbadodecaboran(12)-1-yl]mercury chloride. Methyl*-m-*carboranylmercury chloride. Chloro(methylneobarenyl)mercury. Methylneobarenylmercury chloride*

[23715-64-2]

As Dibromo-μ-1,7-dicarbadodecaboran(12)-1,7-diyldimercury, IC-003321 with

R^1 = —HgCl, R^2 = CH_3

M 393.2

Cryst. (C_6H_6). Mp 251-252°.

Zakharkin, L.I. *et al*, *J. Organomet. Chem.*, 1967, **7**, 385 (*synth*)

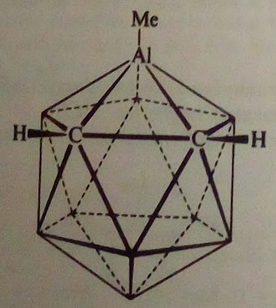
IC-003729

$C_3H_{14}AlB_9$

3-Methyl-3-aluminio-1,2-dicarba-*closo*-dodecaborane(12)

Methyl[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]aluminium

[34540-16-4]



M 174.4

closo-. White cryst. Mp 97-100°. Subl.$_{0.01}$ 90°.

▷ Explodes with water.

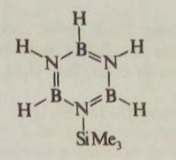
Young, D.A.T. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, ir, pmr, nmr*)

IC-003730

$C_3H_{14}B_3N_3Si$

1-(Trimethylsilyl)borazine, 11CI

[81121-66-6]



M 152.6

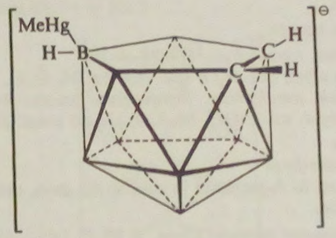
No phys. props. reported.

Nutt, W.R. *et al*, *Inorg. Chem.*, 1982, **21**, 2469 (*synth, props, ms, ir*)

IC-003731

$C_3H_{14}B_9Hg^{\ominus}$

Methyl[(10-η)-undecahydro-7,8-dicarbaundecaborato(2−)]mercurate(1−), 10CI



M 348.0 (ion)

Ph_4As salt: [71788-87-9].

Cryst. (Me_2CO/hexane).

Colquhoun, H.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 619 (*synth, pmr, B-11 nmr, ir*)

IC-003732

$C_3H_{14}B_{10}Hg$

1,2-Dicarbadodecaboran(12)-1-ylmethylmercury, 10CI, 9CI, 8CI

o-Carboranylmethylmercury. Methylmercuri-o-carborane. Methyl(barenyl)mercury. 1-Methylmercurybarene

[20643-85-0]

As Chloro(2-methyl-1,2-dicarbadodecaboran(12)-1-yl)mercury, IC-003727 with

R^1 = —HgMe, R^2 = H

M 358.8

Cryst. (C_6H_6). Mp 200-201°.

Zakharkin, L.J. *et al*, *J. Organomet. Chem.*, 1965, **4**, 211 (*synth*)
Zakharkin, L.J. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 677 (*synth*)
Fedorov, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1970, 798 (*pmr*)
Fedorov, L.A. *et al*, *J. Org. Chem. USSR (Engl. Transl.)*, 1971, **7**, 436 (*pmr*)
Denisovich, L.I. *et al*, *J. Organomet. Chem.*, 1973, **57**, 87 (*electrochem*)
Leites, L.A. *et al*, *Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)
Stanko, V.I. *et al*, *Zh. Obshch. Khim.*, 1978, **48**, 368 (*pmr, B-11 nmr, ir*)

IC-003733

$C_3H_{14}B_{10}Hg$

1,7-Dicarbadodecaboran(12)-1-ylmethylmercury, 10CI, 9CI

1-Methylmercuri-m-*carborane.* (m-*Carboranyl*)*methylmercury. Methyl(neobarenyl)mercury. Methylmercurineobarene*

[27378-33-2]

As Dibromo-μ-1,7-dicarbadodecaboran(12)-1,7-diyldimercury, IC-003321 with

R^1 = —HgMe, R^2 = H

M 358.8

Solid. Mp 169-170°.

Fedorov, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1970, 798 (*pmr, synth*)
Fedorov, L.A. *et al*, *J. Org. Chem. USSR (Engl. Transl.)*, 1971, **7**, 436 (*pmr*)
Stanko, V.I. *et al*, *Zh. Obshch. Khim.*, 1978, **48**, 368 (*pmr, B-11 nmr*)

IC-003734

$C_3H_{14}B_{10}Hg$

1,7-Dicarbadodecaboran(12)-9-ylmethylmercury

(m-*Carboran-9-yl*)*methylmercury. 9-Methylmercuri*-m-*carborane*

[64616-61-1]

As Chloro-1,7-dicarbadodecaboran(12)-9-ylmercury, IC-003342 with

R = —HgMe

M 358.8

Solid.

Zakharkin, L.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1977, 1885 (*synth*)
Grishin, Yu.K. *et al*, *Vestn. Mosk. Univ., Ser. 2: Khim.*, 1982, **23**, 488; *CA*, **98**, 89540v (*Hg-199 nmr*)

IC-003735

$C_3H_{14}B_{10}Hg$

1,12-Dicarbadodecaboran(12)-1-ylmethylmercury, 10CI, 8CI

Methyl(p-*carboranyl*)*mercury. Methylmercuri*-p-*carborane*

[27120-69-0]

As Chloro-1,12-dicarbadodecaboran(12)-2-ylmercury, IC-003343 with

R^1 = —HgMe, R^2 = H

M 358.8

Cryst. (C_6H_6). Mp 192-193°.

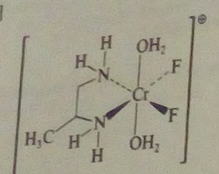
Fedorov, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1970, 798 (*pmr*)
Zakharkin, L.I. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1970, 857 (*synth*)
Fedorov, L.A. *et al*, *J. Org. Chem. USSR (Engl. Transl.)*, 1971, **7**, 436 (*pmr*)
Stanko, V.I. *et al*, *Zh. Obshch. Khim.*, 1978, **48**, 368 (*pmr, B-11 nmr*)

IC-003736

$C_3H_{14}CrF_2N_2O_2^{\oplus}$

Diaquadifluoro(1,2-propanediamine-*N,N'*)chromium(*III*) (1+), 11Cl, 10Cl, 9Cl

[63231-43-6]



M 200.1 (ion)

Struct. not reported.

Chloride: [49634-01-7].
V. hygroscopic purple solid.

Bromide: [40902-39-4].
Purple cryst. + H_2O (H_2O) or pale blue solid on drying.

[94554-17-3]

Vaughn, J.W. *et al, Inorg. Chem.*, 1973, **12**, 2346; 1974, **13**, 598 (*synth*)

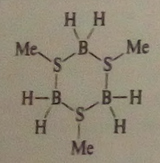
Díaz, C. *et al, Transition Met. Chem.*, 1984, **9**, 469 (*synth, uv-vis, ir*)

IC-003737

$C_3H_{15}B_3S_3$

Hexahydro-1,3,5-trimethylborthiin, 9Cl

1,3,5-Trimethyl-1,3,5,2,4,6-trithiatriborinane. Tris[(methylthio)dihydroborane]



M 179.7

Colourless liq., reasonably stable in air. Sol. THF. d^{20} 1.012. $Bp_{1.5}$ 80-81°.

Monomer:
CH_5BS M 59.9

Mikhailov, B.M. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1962, 1143 (*synth*)

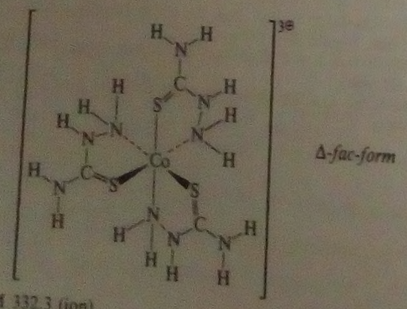
Muetterties, E.L. *et al, Inorg. Chem.*, 1964, **3**, 870 (*synth, ir, pmr*)

IC-003738

$C_3H_{15}CoN_6S_3^{3\oplus}$

Tris(thiosemicarbazide)cobalt(*III*)(3+)

Tris(hydrazinecarbothioamide-N^2,S)cobalt(3+), 11Cl, 10Cl, 9Cl



Δ-fac-form

M 332.3 (ion)

Exists in *fac* and *mer* isomers. Sol. H_2O; v. insol. common org. solvs. Diamagnetic.

▲(±)-*fac-form*
All optically active *cis* isomers eventually racemise.
Violet isomer.

Trichloride: [29855-60-5].
Violet or red cryst. (H_2O).

Trichloride, monohydrate: Pink-lilac needles.

Trichloride, trihydrate: [76771-28-3].
Dark violet cryst. (conc. HCl). Sol. H_2O; spar. sol. org. solvs.

Triiodide, trihydrate: Dark violet, almost black prisms. Sol. H_2O; less readily sol. EtOH and other org. solvs.

Triperchlorate: Violet cryst. Sol. H_2O, MeOH, EtOH; less sol. Et_2O.

Trinitrate, trihydrate: [14263-57-1].
Pale violet plates.

Δ-fac-form
$(-)_D$, cis-*form*

$(+)_D$-*Antimonyl tartrate:* Cryst. + $4H_2O$. $[\alpha]_{589}$ −1290°.

Λ-fac-form
(+)-cis-*form*
Attempts to remove resolving agent were unsuccessful.

$(-)_D$- *Antimonyl tartrate:* Cryst. + $4H_2O$. Sol. H_2O. $[\alpha]_{589}$ +1225°.

(±)-*mer-form*
(±)-*form*
Green isomer.

Trichloride, tetrahydrate: [79854-60-7].
Green cryst. Sol. H_2O; spar. sol. EtOH, Et_2O, Me_2CO.

Tribromide, tetrahydrate: Brown-green prisms. Readily sol. H_2O; spar. sol. EtOH, Me_2CO; almost insol. Et_2O.

Δ-mer-form
(−)-trans-*form*
Converts to Λ-*fac* form in soln. in 15 days, then racemises.

$(+)_D$-*Antimonyl tartrate:* Cryst. + $3H_2O$. $[\alpha]_{589}$ +375°.

Λ-mer-form
(+)-trans-*form*
Converts to Δ-*fac* form and then racemises slowly.

$(-)_D$-*Antimonyl tartrate:* Cryst. + $3H_2O$. $[\alpha]_D$ −375°.

[29855-63-8]

Samus, N.M. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1961, **6**, 1042; 1963, **8**, 35 (*cis and trans salts*)

Sun, K.K.W. *et al, Can. J. Chem.*, 1970, **48**, 2327 (*synth, abs config, optical activity, cd*)

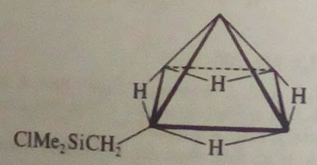
Larsen, E. *et al, Inorg. Chem.*, 1988, **27**, 3051 (*cryst struct, fac-form*)

IC-003739

$C_3H_{16}B_5ClSi$

2-[(Chlorodimethylsilyl)methyl]pentaborane(9), 10Cl

[63838-59-5]



M 169.7

Colourless liq. isolated by vacuum fractionation at −22°.

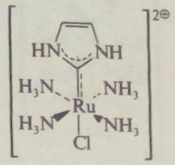
Leach, J.B. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 819 (*nmr, ms, synth*)

IC-003740

$C_3H_{16}ClN_6Ru^{2\oplus}$

Tetraamminechloro(1,3-dihydro-2*H*-imidazol-2-ylidene) ruthenium(2+), 9Cl

Tetraamminechloro(imidazole)ruthenium(III)(2+)



M 272.7 (ion)

trans-Octahedral with imidazole bonded via C(2) in an ylid struct., comparable to a carbene. Sol. H_2O.

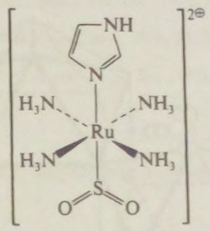
Dichloride: [38118-33-1].
Prepd. by reaction of Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with imidazole, followed by aerial oxidation in aq. HCl. Orange cryst.

Sundberg, R.J. *et al, J. Am. Chem. Soc.*, 1974, **96**, 381 (*synth, uv*)

IC-003741

$C_3H_{16}N_6O_2RuS^{2\oplus}$

Tetraammine(1*H*-imidazole-N^3)(sulfur dioxide-*S*) ruthenium(*II*)(2+); 10Cl



M 301.3 (ion)

trans-Octahedral. Prepd. by treating Tetraamminechloro(sulfur dioxide)ruthenium(*II*)(1+), IC-016432 with imidazole (not always reproducible).

Bis-tetrafluoroborate: [67013-07-4].
Red-brown cryst. Sol. H_2O.

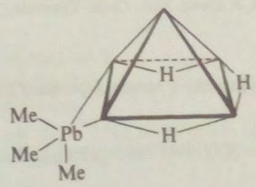
Brown, G.M. *et al, J. Am. Chem. Soc.*, 1978, **100**, 2767 (*synth, uv, pmr, electrochem*)

IC-003742

$C_3H_{17}B_5Pb$

2,3-μ-(Trimethylplumbyl)pentaborane(9), 8Cl

[22142-47-8]



M 314.4

Presumed struct. Unstable liq. Mp −5° dec.

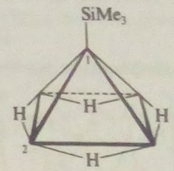
Gaines, D.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 6617.

IC-003743

$C_3H_{17}B_5Si$

1-(Trimethylsilyl)pentaborane(9), 11Cl

[28323-19-5]



M 135.3

Synth. from μ- or 2-$Me_3SiB_5H_8$ at r.t. with Lewis bases such as hexamethylenetetramine or by heating μ-$Me_3SiB_5H_8$ in gas phase at 145°. Liq. purif. by dist. Mp °*ca.* −55.

Gaines, D.F. *et al, Inorg. Chem.*, 1971, **10**, 1094 (*synth, ir, ms, B-11 nmr*)

Gaines, D.F. *et al, Inorg. Chem.*, 1983, **22**, 3155 (*H-2, B-11 nmr*)

IC-003744

$C_3H_{17}B_5Si$

2-(Trimethylsilyl)pentaborane(9), 11Cl

[22142-53-6]

M 135.3

By isom. of 2,3-[μ-(Trimethylsilyl)]pentaborane(9), IC-003745 at r.t. 8h. in Et_2O. Liq., purif. by distillation at −45°. V.p. 1 mm at 0°.

Gaines, D.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 6617 (*synth, ir, ms, pmr, B-11 nmr*)

Gaines, D.F. *et al, Inorg. Chem.*, 1971, **10**, 1094 (*isom*)

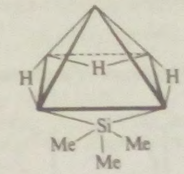
Gaines, D.F. *et al, Inorg. Chem.*, 1983, **22**, 3155 (*H-2, B-11 nmr*)

IC-003745

$C_3H_{17}B_5Si$

2,3-[μ-(Trimethylsilyl)]pentaborane(9), 11Cl

[19553-47-0]



M 135.3

Synth. from LiB_5H_8 and Me_3SiCl in Et_2O at −30°. Liq.; dec. in air; slowly hydrol. by H_2O. Mp 16-17°. V.p. 1 mm at r.t.

Gaines, D.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 6617 (*synth, pmr, ir, ms, B-11 nmr*)

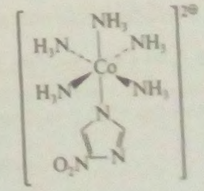
Gaines, D.F., *Inorg. Chem.*, 1971, **10**, 1094 (*isom*)

Gaines, D.F. *et al, Inorg. Chem.*, 1983, **22**, 3155 (*H-2, B-11 nmr*)

IC-003746

$C_3H_{17}CoN_8O_2^{2\oplus}$

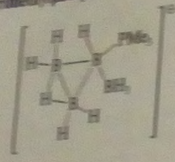
Pentaammine(4-nitro-1*H*-imidazolato-N^3)cobalt(*III*)(2+), 11Cl



M 256.1 (ion)
Dichloride: [84040-88-1]
Bright orange cryst. Sol. H_2O.
Storm, C.B., *Inorg. Chem.*, 1983, **22**, 678 (*synth, cryst struct*)

IC-003747

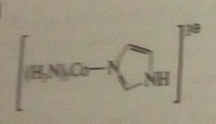
$C_3H_{28}B_9P^{\ominus}$
Nonahydro(trimethylphosphine)octaborate(1−), 11Cl



M 128.3 (ion)
K salt: [85185-84-8].
$C_3H_{28}B_9KP$ M 167.4
Colourless solid, dec. at c.t. Sol. THF.
Shimoi, M. *et al*, *Inorg. Chem.*, 1983, **22**, 1542 (*synth, pmr, B-11 nmr, A-ST nmr*)

IC-003748

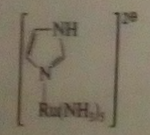
$C_3H_{19}CoN_7^{3\oplus}$
Pentaammine(1*H*-imidazole-*N*^{3})cobalt(*III*)(3+)
[38716-02-8]



M 212.1 (ion)
Triperchlorate: Golden flakes. Sol. DMSO.
N-Ac, triperchlorate: (*1-Acetyl-1H-imidazole-N*^{3})*pentaamminecobalt*(III)(3+) *perchlorate*
Yellow needles (Me_2CO/Et_2O). Sol. Me_2CO.
Harrowfield, J.Mc.B. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 7282 (*synth, uv, pmr, deriv*)

IC-003749

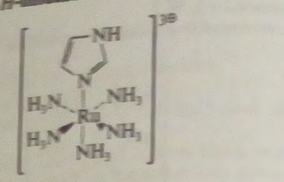
$C_3H_{19}N_7Ru^{2\oplus}$
Pentaammine(1*H*-imidazole-*N*^{3})ruthenium(*II*)(2+), 9Cl
[39003-94-6]



M 254.3 (ion)
Approx. octahedral at Ru, imidazole is bound through N^3.
Prepd. by treating Pentaammine(aqua)ruthenium(*II*) (2+), IC-019980 with imidazole. Sol. H_2O.
Bis-tetrafluoroborate:
Shepherd, R.E. *et al*, *Inorg. Chem.*, 1973, **12**, 1392 (*formn*)
Sundberg, R.J. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 381 (*synth, uv, pmr, electrochem, equation*)
Tweedle, M.F. *et al*, *Inorg. Chem.*, 1982, **21**, 3361 (*imm, reaction, electrochem*)
Nocera, D.G. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5145 (*electron-transfer*)
Jackman, M.P. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5880 (*electron-transfer*)

IC-003750

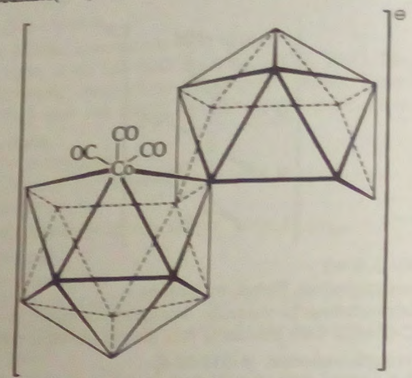
$C_3H_{19}N_7Ru^{2\oplus}$
Pentaammine(1*H*-imidazole-*N*^{3})ruthenium(*III*)(3+), 9Cl



M 254.3 (ion)
Sol. H_2O.
Trichloride: [51982-73-1].
$C_3H_{19}Cl_3N_7Ru$ M 360.6
Prepd. by reaction of Pentaammine(aqua)ruthenium(*II*) (2+), IC-019980 with an excess of imidazole, followed by aerial oxidation in aq. HCl. pK_a 8.9 (N^1).
Sundberg, R.J. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 381 (*synth, uv, electrochem, pK_a*)

IC-003751

$C_3H_{20}B_{18}CoO_3^{\ominus}$
Tricarbonyl[(6,7,8,9-η)-eicosahydrodecaborano(14)[6′,7′:5,6]decaborato(2−)]cobaltate(1−)



2H not shown

M 357.7 (ion)
Me_4N salt: [36182-41-9].
Synth. from Na(*anti*-$B_{18}H_{20}$) and $Co_2(CO)_8$ in dry THF. Red-brown cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2.
Todd, L.J. *et al*, *Inorg. Chem.*, 1973, **12**, 44 (*synth, ir, uv-vis, B-11 nmr*)
Todd, L.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1990, 693.

IC-003752

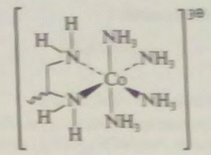
$C_3H_{21}CoN_7^{3\oplus}$
Pentaammine(dimethylcyanamide)cobalt(*III*)(3+), 11Cl
[87450-94-0]

$[Co(N{\equiv}CNMe_2)(NH_3)_5]^{3\oplus}$

M 214.1 (ion)
Hydrol. by base.
Triperchlorate: Sol. H_2O, DMSO.
Dixon, N.E. *et al*, *Inorg. Chem.*, 1983, **22**, 4038 (*synth, uv, pmr, cmr, kinetics*)

IC-003753

$C_3H_{22}CoN_4^{3\oplus}$
Tetraammine(1,2-propanediamine-*N,N′*)cobalt(3+)
Tetraammine-(1,2-diaminopropane)cobalt(III)
[22330-29-6]



M 201.1 (ion)
Compds. with *R* or *S* ligands have been separately studied.
Trichloride: [15279-21-7].
$C_3H_{22}Cl_3CoN_4$ M 307.5
Orange plates (EtOH aq.).
Triperchlorate: [76484-71-4].
Yellow cryst. ($HClO_4$ aq.).
[22330-30-9, 23311-41-3, 34876-45-4, 58452-10-1, 81314-14-9, 81314-16-1]
Hawkins, C.J. *et al*, *Acta Chem. Scand.*, 1965, **19**, 1915 (*synth, cd*)
Buckingham, D.A. *et al*, *Aust. J. Chem.*, 1967, **20**, 257 (*pmr, conformn*)
Ogino, K. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 351 (*cd*)
Yoneda, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 2863 (*synth, pmr*)
Hawkins, C.J. *et al*, *Aust. J. Chem.*, 1976, **29**, 33; 1981, **34**, 2505 (*synth, pmr, cryst struct*)
Gainsford, A.R. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 792 (*synth, pmr*)

IC-003754

$C_3H_{22}CoN_7O^{2\oplus}$
Pentaammine(*N,N*-dimethylureato-*N*′)cobalt(*III*)(2+), 11Cl
[87450-95-1]

$[Co(NHCONMe_2)(NH_3)_5]^{2\oplus}$

M 231.1 (ion)
Bis-trifluorosulfonate: Red cryst. Sol. DMSO.
Dixon, N.E. *et al*, *Inorg. Chem.*, 1983, **22**, 4039 (*synth, uv, pmr, cmr*)

IC-003755

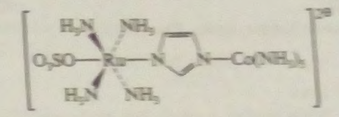
$C_3H_{24}CoN_5O_4P^{3\oplus}$
Pentaammine(trimethylphosphate-*O*‴)cobalt(*III*)(3+), 10Cl
[14970-17-3]

$[Co(NH_3)_5O{=}P(OMe)_3]^{3\oplus}$

M 284.1 (ion)
Triperchlorate: [15041-41-5].
Pink cryst. Sol. H_2O.
▷ Potentially explosive.
Schmidt, W., *Inorg. Chem.*, 1963, **2**, 698 (*synth, reactions*)
Dixon, N.E. *et al*, *Inorg. Chem.*, 1981, **20**, 470 (*synth, uv, pmr*)

IC-003756

$C_3H_{28}CoN_{11}O_9RuS^{2\oplus}$
Tetraammine[μ-(1*H*-imidazolato-*N*^{1}:*N*^{3})][pentaamminecobalt][sulfato(2−)-*O*]ruthenium(2+), 10Cl
Pentaamminecobalt(III)-μ-*imidazolato*(*tetraammine*)*sulfatoruthenium*(II)



M 476.4 (ion)
trans-Configuration at Ru.
Bis-tetrafluoroborate: [68447-56-3].
Sol. H_2O.
Isied, S.S. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 6754 (*synth, uv, electrochem*)

IC-003757

$C_3HgN_3^{\ominus}$
Tris(cyano-*C*)mercurate(1−)
[19426-08-5]

$[Hg(CN)_3]^{\ominus}$

M 278.6 (ion)
Cs salt: [53536-23-5].
Obt. by evap. of MeOH solns. of CsCN and $Hg(CN)_2$. Cryst. Anions form tetrahedra, linked into chains via sharing of 2-corners.
Thiele, G. *et al*, *Naturwissenschaften*, 1974, **61**, 215 (*synth, cryst struct, Cs salt*)
Chadwick, B.M. *et al*, *J. Mol. Struct.*, 1980, **63**, 467 (*synth, ir, raman, Cs salt*)
Kirowa-Eisner, E. *et al*, *Anal. Chem.*, 1981, **53**, 581 (*stability const*)

IC-003758

$C_3HgN_3O^{\ominus}$
Bis(cyano-*C*)(cyanato-*O*)mercurate(1−)

$[Hg(CN)_2OCN]^{\ominus}$

M 294.6 (ion)
Na salt, dihydrate: [73887-53-3].
Colourless platelets (H_2O). Strong linear Hg—CN bonds with weaker 2HgO and 2HgN bonds.
K salt: [73887-51-1].
Colourless prisms (H_2O). Strong linear Hg—CN bonds with weaker 4HgN.
Rb salt: [73887-49-7].
Cryst. (H_2O).
Cs salt: [73887-47-5].
Platelets + $1H_2O$ (H_2O). 2 Strong Hg—CN bonds: weaker Hg connections to 4NCO units.
Thiele, G. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **461**, 109 (*synth, ir, raman, cryst struct*)

IC-003759

$C_3HgN_3O_3^{\ominus}$
Tris(cyanato-*N*)mercurate(1−)

$[Hg(NCO)_3]^{\ominus}$

M 326.6 (ion)
Struct. of salts can be considered to be made up of $Hg(OCN)_2$, $OCN^{\ominus}$ and $M^{\oplus}$ ions because Hg forms linear short bonds to 2 OCN and longer bonds to 4 NCO groups.
K salt: [28459-59-8].
White cryst.

Rb salt: [65450-38-6].
White cryst.
[38722-88-2]
Thiele, G. *et al*, *Z. Naturforsch., B*, 1977, **32**, 1239 (*synth, ir, raman, cryst struct, K and Rb salt*)

IC-003760

$C_3HgN_3S^{\ominus}$
Bis(cyano-*C*)(thiocyanato-*S*)mercurate(1 −)
$[Hg(SCN)(CN)_2]^{\ominus}$

M 310.7 (ion)
Na salt: White needles $+1H_2O$. Sol. H_2O; insol. EtOH. Mp >250°. Dehydrates at 110°.
K salt: [73596-74-4].
Cryst.
Rb salt: [73596-78-8].
Salt.
Cs salt: [73596-80-2].
Cryst.
Tetraaquamagnesium salt (2:1): [87506-87-4].
Cryst. Two Hg octahedral environments in solid: Hg(1): 2O + 2C + 3S, Hg(2): 4S + 2C.
Tetraaquacalcium salt (2:1): [87506-88-5].
Cryst.
Tetraaquastrontium salt (2:1): [87506-90-9].
Cryst. Struct. contains octahedral Hg (4S + 2C) and 9-coord. Sr (5N + 4O).
Tetraaquabarium salt (2:1): [87506-92-1].
Cryst.

Agrawal, A.K. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **312**, 230; 1965, **336**, 66 (*synth, K and Na salts*)
Agrawal, A.K. *et al*, *J. Prakt. Chem.*, 1968, **310**, 119 (*ir, Na and K salts*)
Thiele, G. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **461**, 109 (*synth, ir, cryst struct, alkali metal salts*)
Brodersen, K. *et al*, *Z. Anorg. Allg. Chem.*, 1983, **500**, 171 (*synth, cryst struct, $[M(OH_2)_4]$ salts*)

$C_3HgN_3S_3^{\ominus}$ IC-003761
Tris(thiocyanato-*S*)mercurate(1 −)
Trithiocyanatomercurate(1 −)
[21667-89-0]
$[Hg(SCN)_3]^{\ominus}$

M 374.8 (ion)
K salt: [52139-52-3].
Rb salt: [52139-53-4].
Cs salt: [52139-54-5].
Cryst. Struct. comprises dimeric units $[Hg_2(SCN)_6]$: 2 edge-linked tetrahedra; $Cs^{\oplus}$ occupies spaces between anions.
NH_4 salt: [52139-51-2].
Ph_4P salt: [53516-71-5].
Cryst. Infinite chains of $[Hg(SCN)_3]^{\ominus}$ are bridged by SCN: tetrahedral Hg.
[Bis(ethylenedithiolato)tetrathiafulvalene]$_3$(1+) salt: [123341-63-9]. *Tris[2-(5,6-dihydro-1,3-dithiolo[4,5-b][1,4]dithiin-2-ylidene)-5,6-dihydro-1,3-dithiolo[4,5-b]dithiin] (1+) salt*
Cryst. Metal/insulator transition occurs at *ca.* 180K.

Larbot, A. *et al*, *Rev. Chim. Miner.*, 1973, **10**, 465 (*synth, ir, NH_4, Cs, K and Rb salts*)
Thiele, G. *et al*, *Naturwissenschaften*, 1974, **61**, 215 (*synth, cryst struct, Cs salt*)
Sakhri, A. *et al*, *Inorg. Chem.*, 1975, **14**, 740 (*synth, cryst struct, Ph_4P salt*)
Brown, R.J. *et al*, *CA*, 1983, **99**, 166114 (*raman*)

Ahrland, S. *et al*, *Acta Chem. Scand., Ser. A*, 1985, **39**, 227 (*stability const in Py*)
Oshima, M. *et al*, *Chem. Lett.*, 1989, 1159 (*synth*)

IC-003762

$C_3HoN_3S_3$
Holmium(*III*) thiocyanate
$Ho(NCS)_3$

M 339.1
Synth. by metathesis and used as soln.
Hexahydrate: Hygroscopic yellow cryst. Sol. EtOH, H_2O. Probably contains $Ho(NCS)_3(OH_2)_5$ molecules.

Vincentini, G. *et al*, *Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al*, *Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110 (*ir*)

IC-003763

C_3IIrO_3
Tricarbonyliodoiridium
$IrI(CO)_3$

M 403.1
Possibly polymeric. Useful starting material for iridium iodo-carbonyl complexes. Brown solid. Ir ν_{CO} 2073, 2046 cm^{-1} (nonanoic acid). One-dimensional conductor.

Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1941, **246**, 138 (*synth*)
Forster, D., *J. Chem. Soc., Dalton Trans.*, 1979, 1639 (*synth, ir*)

$C_3INiO_3^{\ominus}$ IC-003764
Tricarbonyliodonickelate(1 −), 9CI, 8CI
Iodotricarbonylnickelate(1 −)
[36830-71-4]
$[Ni(CO)_3I]^{\ominus}$ (C_{3v})

M 269.6 (ion)
Catalyst for carbonylation of benzyl chloride and carbonylation with acetylene insertion of acyl halides. Anion stable in air-free soln. even at 70-80°.
Na salt: [27122-29-8].
$C_3INaNiO_3$ M 292.6
Not stable in the pure state.
Tetrabutylammonium salt: [27122-27-6].
Not stable in pure state.

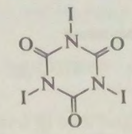
Cassar, L. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 291 (*synth, ir*)
Foa, M. *et al*, *Gazz. Chim. Ital.*, 1972, **102**, 85 (*synth, use*)

C_3IO_3Rh IC-003765
Tricarbonyliodorhodium, 9CI
Iodotris(carbonyl)rhodium
[40784-47-2]
$Rh(CO)_3I$

M 313.8
Unstable in the absence of a high CO pressure. Ir ν_{CO} 2084, 2054 cm^{-1} (hexane).

Morris, D.E. *et al*, *J. Organomet. Chem.*, 1973, **49**, C53 (*synth, ir*)

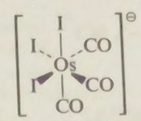
$C_3I_3N_3O_3$ IC-003766
1,3,5-Triiodo-1,3,5-triazine-2,4,6-trione
Triiodoisocyanuric acid
[59104-32-4]



M 506.7
Formed by polym. of Iodine isocyanate, IC-002718. Orange-red powder, more stable than Cl and Br analogues. Rapidly hydrol. by H_2O. Sl. sol. Me_2CO, MeCN.

Gottardi, W., *Monatsh. Chem.*, 1970, **101**, 655 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1976, **D3**, 147 (*bibl*)

$C_3I_3O_3Os^{\ominus}$ IC-003767
Tricarbonyltriiodoosmate(1 −), 9CI



fac-form

M 654.9 (ion)
fac-form
Tetrabutylammonium salt: [55399-59-2].
Bright-yellow cryst. (EtOH).
mer-form
Tetrabutylammonium salt: [58776-25-3].
Yellow.

Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Preetz, W. *et al*, *J. Organomet. Chem.*, 1975, **86**, 397; 1976, **104**, 79 (*synth, ir, raman*)

$C_3I_3O_3Ru^{\ominus}$ IC-003768
Tricarbonyltriiodoruthenate(1 −), 8CI
[32423-83-9]
As Tribromotricarbonylruthenate(1 −), IC-003524 with
X = I

M 565.8 (ion)
Cs salt: [22594-83-8].
$C_3CsI_3O_3Ru$ M 698.7
Yellow cryst.
Et_4N salt: [83721-25-9].
Yellow cryst. (MeOH).

Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Colton, R. *et al*, *Aust. J. Chem.*, 1971, **24**, 903 (*synth, ir*)
Dombek, B.D. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 6508 (*synth, use*)
Dykstra, R.W. *et al*, *J. Magn. Reson.*, 1982, **46**, 338 (*nmr*)
Hidai, M. *et al*, *Organometallics*, 1983, **2**, 292 (*synth*)

C_3InN_3 IC-003769
Indium(*III*) cyanide
Indium tricyanide
$In(CN)_3$

M 192.8
Synth. from $(CN)_2$ and InOI at 300°. White deliquescent cryst. V. sol. H_2O. Sol. EtOH, Me_2CO, Et_2O. Insol. C_6H_6, CCl_4. Subl. 340-350°. Slow hydrol. in aq. soln.

Goggin, P.L. *et al*, *J. Chem. Soc. A*, 1966, 1314 (*synth, powder struct*)

$C_3InN_3S_3$ IC-003770
Indium(*III*) thiocyanate
[60131-22-8]
$In(SCN)_3$

M 289.0
Synth. from NaSCN and $InCl_3$ in EtOH. White deliquescent cryst. (MeOH). Spar. sol. xylene, C_6H_6, CCl_4. Sol. EtOH, Me_2CO, Et_2O. Dec. >150°. Slow hydrol. in aq. soln. Many complexes $In(SCN)_3L_3$ formed with unidentate N- or O-donor L.

Goggin, P.L. *et al*, *J. Chem. Soc. A*, 1966, 1314 (*synth, powder struct*)
Patel, S.J. *et al*, *J. Chem. Soc. A*, 1967, 1187 (*synth, ir, complexes*)

$C_3LaN_3S_3$ IC-003771
Lanthanum(*III*) thiocyanate
$La(NCS)_3$

M 313.1
Usually not isol.; synth. by metathesis and used in soln.
Heptahydrate: [102563-34-8].
Hygroscopic colourless cryst. Sol. H_2O, EtOH. Contains $La(NCS)_3(OH_2)_6$ molecules, one H_2O molecule uncoord. 9-Coord., capped square antiprism. Cd-Nd analogues known.
Tetrakis-HMPA complex: [53781-31-0].
$C_{27}H_{72}LaN_{15}O_4P_4S_3$ M 1029.9
Colourless cryst. + ½ toluene. Sol. toluene, C_6H_6. Mp 183-185°. Contains N-bonded thiocyanate.

Cleve, P.T., *Bull. Soc. Chim. Fr.*, 1874, **21**, 190 (*synth*)
O'Neill, L. *et al*, *Trans. Faraday Soc.*, 1934, **30**, 1134 (*synth*)
Vincentini, G. *et al*, *Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth, ir*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al*, *Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*synth, ir*)
Zhu, N. *et al*, *New Front. Rare Earth Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304; *CA*, 1986, **105**, 70454 (*cryst struct*)
Barr, D. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1990, **29**, 285 (*synth, cryst struct, pmr, HMPA complex*)

$C_3La_2O_9$ IC-003772
Lanthanum carbonate ($La_2(CO_3)_3$)
[587-26-8]
$La_2(CO_3)_3$

M 457.8
Colourless cryst. Stable to 400-440°; ultimately dec. to La_2O_3 on heating.
Octahydrate: [6487-39-4].
When also containing Ce, forms mineral Lanthanite, $(La,Ce)_2(CO_3)_3.8H_2O$. Colourless cryst. Possesses irregular layer struct. with two diff. 10-coord. sites- La(1) bound to $4H_2O$, two monodentate CO_3, two bidentate CO_3; La(2) bound to $2H_2O$, four bidentate CO_3.
[14519-91-6, 54451-24-0, 64340-75-6]

Salustry, M.L. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3306 (*synth*)

Caro, P.E. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **267**, 1594; 1969, **269**, 687 (*synth*)
Shim, D.B. *et al, Inorg. Chem.*, 1968, **7**, 1340 (*cryst struct*)
Wakita, H. *et al, Bull. Chem. Soc. Jpn.*, 1972, **45**, 2476; 1973, **46**, 152 (*synth, ir, dta, tga, struct*)
Caro, P.E. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 1167 (*synth, ir*)
Firsching, F.H. *et al, J. Chem. Eng. Data*, 1986, **31**, 40 (*sol*)

IC-003773

$C_3LuN_3S_3$

Lutetium(*III*) thiocyanate

$Lu(NCS)_3$

M 349.2
Synth. by metathesis and used as soln.
Hexahydrate: Hygroscopic colourless cryst. Sol. H_2O, EtOH. Prob. 8-coord., containing $Lu(NCS)_3(OH_2)_5$ molecules.

Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*ir*)

IC-003774

$C_3MnNO_4^{3\ominus}$

Tricarbonylnitrosylmanganate(2 –), 11Cl

[84928-58-5]

$[(OC)_3MnNO]^{2\ominus}$

M 168.9 (ion)
Di-Na salt, bis-crypt[2.2.2] complex: [84928-59-6].
Synth. by treatment of $Mn(NO)(CO)_3(PPh_3)$ with Na/Hg in THF at r.t. followed by addition of cryptand (2.2.2). Light-yellow cryst. Ir ν_{CO} 1840s, 1720vs; ν_{NO} 1480m cm^{-1}.
Di-K salt: [84928-56-3].
Yellow microcryst. Ir ν_{CO} 1900m, 1755vs; ν_{NO} 1420s cm^{-1} (THF).
[84928-57-4]

Chen, Y.-S. *et al, J. Am. Chem. Soc.*, 1983, **105**, 1689 (*synth, ir*)

IC-003775

C_2N_2O

Carbonyl cyanide

Oxopropanedinitrile, 9Cl. Mesoxalic dinitrile. Mesoxalonitrile

[1115-12-4]

NCCOCN

M 80.0
Formed from tetracyanoethylene oxide + dibutyl sulfide. Cyanoformylating reagent, also capable of Diels-Alder reactions. Colourless liq. d_4^{20} 1.124. Fp –36° to –35°, Mp –37.9°. Bp_{748} 65.5°, Bp 67°. Burns with bright-violet flame. Has overpowering odour reminiscent of HCN.

▷ Reacts explosively with H_2O, vigorously with alcohols.

Malachowski, R. *et al, Ber.*, 1937, **70**, 1012; 1938, **71**, 2239 (*synth*)
Linn, W.J. *et al, J. Am. Chem. Soc.*, 1965, **87**, 3651 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 60
Bates, J.B. *et al, Spectrochim. Acta, Part A*, 1969, **26**, 455 (*microwave*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1971, **D1**, 381 (*bibl*)
Org. Synth., 1971, **51**, 70 (*synth*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 455.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 472.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 384.

IC-003776

$C_3N_3NdS_3$

Neodymium(*III*) thiocyanate

$Nd(NCS)_3$

M 318.4
Synth. by metathesis and used in soln.
Heptahydrate: Hygroscopic lilac cryst. Contains tricapped square antiprismatic $Nd(NCS)_3(OH_2)_6$ molecules, with one H_2O uncoord.

Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*ir*)
Zhu, N. *et al, New Front. Rare Earth Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304; *CA*, 1986, **105**, 70454 (*cryst struct*)

IC-003777

$C_3N_3Ni^{2\ominus}$

Tris(cyano-*C*)nickelate(2 –), 9Cl

Tricyanonickelate(I)(*2 –*)

[52488-77-4]

$[Ni(CN)_3]^{2\ominus}$

M 136.7 (ion)
Compds. with this formula are almost certainly salts of Hexakis(cyano-*C*)dinickelate(4 –), IC-005606.
Di-K salt: [39049-81-5].
$C_3K_2N_3Ni$ M 214.9

Nag, K. *et al, Coord. Chem. Rev.*, 1980, **33**, 87.

IC-003778

$C_3N_3NiS_3^{2\ominus}$

Tris(thiocyanato-*N*)nickelate(*II*)(2 –), 9Cl

Tris(isothiocyanato)nickelate(II)(*2 –*).
Triisothiocyanatonickelate(II)(*2 –*)

$[Ni(NCS)_3]^{2\ominus}$

M 232.9 (ion)
Salts of alkali metals thought to be dinuclear $[Ni_2(NCS)_6]^{4\ominus}$.
Tributylphosphonium salt: [62598-21-4].
Orange-brown solid. Mp 205-206° dec. Anion may have octahedral polymeric struct.

Kharitonov, Y.Y. *et al, Inorg. Nucl. Chem. Lett.*, 1970, **6**, 201.
Alyea, E.C. *et al, J. Coord. Chem.*, 1976, **5**, 143.

IC-003779

C_3N_3OP

Phosphoryl cyanide, 8Cl

Phosphorus(V) *oxytricyanide. Tricyanooxophosphorus*(V). *Tricyanophosphine oxide*

[34217-67-9]

$P(O)(CN)_3$

M 125.0
Obt. by oxidation of Phosphorus cyanide, IC-003785 with nitrogen oxides or pyridine-*N*-oxide. Phys. props not recorded.

Goubeau, J. *et al, Spectrochim. Acta, Part A*, 1971, **27**, 1703 (*ir*)
Albrecht, S. *et al, Z. Anorg. Allg. Chem.*, 1987, **552**, 132 (*synth, props, P-31 nmr*)

IC-003780

$C_3N_3OPS_3$

Phosphoryl isothiocyanate, 9Cl

Triisothiocyanatooxophosphorus(V)

[1858-25-9]

$(SCN)_3P{=}O$

M 221.2
Liq. $Bp_{0.5}$ 106-107°, $Bp_{0.05}$ 119°. V. reactive to protic substances.

Sowerby, D.B., *J. Inorg. Nucl. Chem.*, 1961, **22**, 205 (*synth, ir*)
Fluck, E. *et al, Z. Anorg. Allg. Chem.*, 1965, **338**, 58 (*synth, P-31 nmr*)
Pudovik, A.N. *et al, Zh. Obshch. Khim.*, 1979, **49**, 1425; *J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 1248 (*synth, ir, P-31 nmr*)

IC-003781

$C_3N_3OS_3Zr^{\ominus}$

Oxotris(thiocyanato-*N*)zirconate(*IV*)(1 –), 11Cl

Oxotri(isothiocyanato)zirconate(IV)(*1 –*)

$[(SCN)_3Zr{=}O]^{\ominus}$

M 281.4 (ion)
May be oligomeric.
Cs salt: [98912-87-9].
White solid + $2H_2O$.
Pyridinium salt: White solid + $2H_2O$.

Khariyonov, Yu.Ya. *et al, Izv. Akad. Nauk SSSR Neorg. Mat.*, 1962, 402; *CA*, **57**, 8163e (*synth, ir*)
Perek, M., *Inorg. Chim. Acta*, 1985, **103**, 163 (*ir, raman*)

IC-003782

$C_3N_3O_2S_3U^{\ominus}$

Dioxotris(thiocyanato-*N*)uranate(*VI*)(1 –)

Tris(isothiocyanato)dioxouranate(VI)(*1 –*)

[36423-13-9]

$[UO_2(NCS)_3]^{\ominus}$

M 444.2 (ion)
K salt: [74171-91-8].
Orange-red cryst. + $2H_2O$. Sol. H_2O, Et_2O, Me_2CO, MeOH, EtOH. Loses H_2O on heating to 125°.
Rb salt: Orange-red cryst. + $2H_2O$. Sol. MeOH, EtOH, H_2O, Me_2CO, Et_2O. Loses H_2O on heating to 140°.
NH_4 salt: Yellow cryst. + $2H_2O$. Sol. H_2O, Et_2O, Me_2CO, MeOH, EtOH. Loses H_2O on heating to 140°.

Markov, V.P. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1960, **5**, 724 (*synth*)
Volovenko, V.M. *et al, Radiokhimiya*, 1967, **9**, 119 (*synth*)
Volovenko, V.M. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1577 (*synth*)

IC-003783

$C_3N_3O_3P$

Phosphorous triisocyanate, 9Cl

Tris(isocyanato)phosphorus(III). *Phosphorus isocyanate, 8Cl. Trisocyanatophosphine*

[1782-09-8]

$P(NCO)_3$

M 157.0
Synth. from PCl_3 + AgNCO in C_6H_6. Ligand for Ti, Zr. Colourless liq. V. reactive to H_2O and other protic reagents. Apparently polym. on standing but depolymerised at 80°/25 mm. d 1.44. Mp –2°. Bp 169°. n_D 1.5352.

▷ Irritant to nose and eyes.

Oxide: see *Phosphoryl isocyanate, IC-003784*

Forbes, G.S. *et al, J. Am. Chem. Soc.*, 1940, **62**, 761 (*synth*)
Miller, F.A. *et al, Spectrochim. Acta*, 1963, **18**, 1311 (*synth, str, ir, raman*)
Fluck, E., *Z. Naturforsch., B*, 1964, **19**, 869 (*P-31 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 622 (*rev, bibl*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 584 (*rev*)
Dimond, R.J. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 1455 (*anal, reactions*)
Dillon, K.B. *et al, Phosphorus Sulfur*, 1984, **19**, 299 (*reactions*)

IC-003784

$C_3N_3O_4P$

Phosphoryl isocyanate, 9Cl

Triisocyanatooxophosphorus(V)

[1858-24-8]

$(OCN)_3P{=}O$

M 173.0
Liq. Mp 5°, Bp 193°, Bp_{18} 88°. Highly reactive to protic substances.

Miller, F.A. *et al, Spectrochim. Acta*, 1963, **18**, 1311 (*synth, ir, raman*)
Fluck, E., *Z. Naturforsch., B*, 1964, **19**, 869 (*P-31 nmr*)
Borovikov, Yu.Ya. *et al, Zh. Obshch. Khim.*, 1975, **45**, 2377; *J. Gen. Chem. USSR (Engl. Transl.)*, 1975, **45**, 2335 (*struct*)

IC-003785

C_3N_3P

Phosphorus cyanide, 8Cl

Phosphorous tricyanide, 9Cl. Tricyanophosphine. Tricyanophosphorus(III)

[1116-51-4]

$P(CN)_3$

M 109.0
Tetragonal. Pyramidal struct. Interatomic distances: P—C 178, C—N 115 pm; angles: CPC 93°, PCN 172°. Dimeric in dioxan, MeCN and C_6H_6. Tetrameric in $MeNO_2$. Synth. from PCl_3 or PBr_3 + AgCN in CCl_4. V. hygroscopic, flat needles and platelets. Sl. sol. $CHCl_3$, CS_2, PCl_3, Et_2O. Mp *ca.* 200°. $Subl_{0.1}$ 50-60°. Reacts readily with H_2O. Burns if heated in dry air.

Inorg. Synth., 1960, **6**, 84 (*synth, props*)
Emerson, K. *et al, Acta Crystallogr.*, 1964, **17**, 1134 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, **C**, 621 (*rev, bibl*)
Kirk, P.G. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 892 (*props, ir*)
Coulcran, K.J. *et al, Inorg. Chem.*, 1971, **10**, 1536 (*synth, ir, ms, P-31 nmr*)
Cyvin, S.J. *et al, J. Mol. Struct.*, 1973, **17**, 371 (*struct, spectra*)
Edwards, H.G.M. *et al, Spectrochim. Acta, Part A*, 1976, **32**, 731; 1987, **43**, 1345 (*synth, raman*)
Elbel, S. *et al, Z. Naturforsch., B*, 1976, **31**, 1472 (*pe*)
Delgado, M.S. *et al, Z. Anorg. Allg. Chem.*, 1980, **467**, 225 (*complexes*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2777 (*haz*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th Ed., Butterworth, London and Boston, 1990, 406 (*haz*)

IC-003788

$C_3N_3PS_3$

Phosphorous trüsothiocyanate, 9Cl

Phosphorus isothiocyanate, 8Cl. Tris(thiocyanato-N) phosphorus (III)

[1858-23-7]

$P(NCS)_3$

M 205.2

Synth. from PCl_3 + $Pb(SCN)_2$, or from BCl_3 + Me_3SiNCS, or from PCl_3 + $MSCN$ (M = Na, K, NH_4). Colourless, highly refractive liq. Extremely reactive to H_2O and other protic reagents. d_4^{15} 1.483. Mp −4°. Bp_{15-17} 163-168° dec., Bp 118-120°, $Bp_{0.04}$ 75°. Polym. and dec. above 105°.

Oxide: see *Phosphoryl isothiocyanate, IC-003780*

Sowerby, D.B., *J. Inorg. Nucl. Chem.*, 1961, **22**, 205 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 632 (*rev, bibl*)
Fluck, E. *et al, Z. Anorg. Allg. Chem.*, 1965, **338**, 52; 1967, **354**, 139 (*synth, reactions, P-31 nmr*)
Oba, K. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 1515 (*synth, ir, raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 590 (*rev*)
Pudovik, A.N. *et al, Zh. Obshch. Khim.*, 1979, **49**, 1425; *J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 248 (*synth, P-31 nmr*)
Krupoder, S.A. *et al, J. Fluorine Chem.*, 1983, **22**, 305 (*pe*)

$C_3N_3PrS_3$ IC-003787

Praseodymium(*III*) thiocyanate

$Pr(NCS)_3$

M 315.1
Normally not isol.; synth. by metathesis and used in soln.
Heptahydrate: [38785-80-7].
Hygroscopic green cryst. Contains mono-capped tetragonal antiprism $Pr(NCS)_3(H_2O)_4$ molecules, with one H_2O uncoord. Isostructural with La-Eu analogues.

Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 723 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Lazarev, P.I. *et al, Zh. Strukt. Khim.*, 1972, **13**, 543; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1972, **13**, 507 (*synth, cryst struct*)
Lazarev, P.I. *et al, Koord. Khim.*, 1975, **1**, 979; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1975, **1**, 830
Zhu, N. *et al, New Front. Rare Earth Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304; *CA*, 1986, **105**, 70454 (*synth, cryst struct*)

C_3N_3Rh IC-003788

Rhodium(*III*) cyanide ($Rh(CN)_3$)
Rhodium tricyanide

$Rh(CN)_3$

M 180.9
Trihydrate: Rhodium(III) *cyanide trihydrate*
$C_3H_4N_3O_3Rh$ M 235.0
Prepared from $RhCl_3.3H_2O$ and KCN. Yellow powder.

Lawson, D.N. *et al, J. Chem. Soc. A*, 1966, 52 (*synth, ir*)

$C_3N_3S_3Sm$ IC-003789

Samarium(*III*) thiocyanate

$Sm(NCS)_3$

M 324.6
Generally synth. by metathesis and used as soln.
Hexahydrate: [102512-23-2].
Hygroscopic yellow cryst. Sol. H_2O. One H_2O uncoord.. Contains sq. antiprismatic $Sm(NCS)_3(OH_2)_5$ molecules. Sm→Gd form isomorphous compds.
Heptahydrate: Yellow cryst. Isomorphous with other rare earth heptahydrates.

Cleve, P.T., *Bull. Soc. Chim. Fr.*, 1885, **43**, 166 (*synth*)
Ephraim, R., *Chem. Ber.*, 1929, **62**, 1639 (*uv-vis*)
Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*ir*)
Lazarev, P.I. *et al, Koord. Khim.*, 1975, **1**, 979; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1975, **1**, 830 (*struct*)
Zhu, N. *et al, New Front. Rare Earth Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304; *CA*, 1986, **105**, 70454 (*cryst struct*)

$C_3N_3S_3Tb$ IC-003790

Terbium(*III*) thiocyanate

$Tb(NCS)_3$

M 333.1
Synth. by metathesis and used in soln.
Hexahydrate: Hygroscopic pale pink cryst. Sol. H_2O, EtOH. Probably 8-coord. containing $Tb(NCS)_3(OH_2)_5$ molecules.

Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*ir*)

$C_3N_3S_3Tm$ IC-003791

Thulium(*III*) thiocyanate

$Tm(NCS)_3$

M 343.1
Synth. by metathesis and used as soln.
Hexahydrate: Hygroscopic green cryst. Sol. EtOH, H_2O. Presumed 8-coord. by analogy with Eu, Gd, Y compds., with one H_2O uncoord.

Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)

$C_3N_3S_3Y$ IC-003792

Yttrium(*III*) thiocyanate

$Y(NCS)_3$

M 263.1
Not usually isol.; prep. by metathesis and used in soln.
Hexahydrate: [102512-25-4].
Hygroscopic colourless cryst. Sol. H_2O. 8-Coord. square antiprismatic at Y, one H_2O uncoord.
Tris-HMPA complex: [54092-04-5].
$C_{21}H_{54}N_{12}O_3P_3S_3Y$ M 800.7
Colourless cryst. Sol. toluene. Mp 177-199°. Prob. 6-coord. octahedral complex.

Cleve, P.T. *et al, Bull. Soc. Chim. Fr.*, 1872, **18**, 198 (*synth*)
Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth, ir*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*ir*)
Zhu, N. *et al, New Front. Rare Earth Sci. Appl., Proc. Int. Conf. Rare Earth Dev. Appl.*, 1985, **1**, 304; *CA*, 1986, **105**, 70454 (*cryst struct*)
Barr, D. *et al, Angew. Chem., Int. Ed. Engl.*, 1990, **29**, 285 (*synth, HMPA complex*)

$C_3N_3S_3Yb$ IC-003793

Ytterbium(*III*) thiocyanate

$Yb(NCS)_3$

M 347.2
Synth. by metathesis and used in soln.

Hexahydrate: Colourless hygroscopic cryst. Sol. EtOH, H_2O. Presumed 8-coord. by analogy with Eu, Gd, Y compds., with one H_2O uncoord.

Vincentini, G. *et al, Ann. Acad. Bras. Cienc.*, 1964, **36**, 123 (*synth*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 579 (*synth*)
Kawamura, K. *et al, Trans. Natl. Res. Inst. Met. (Jpn.)*, 1965, **7**, 110; 1966, **8**, 10 (*ir*)

C_3N_3V IC-003794

Vanadium(*III*) cyanide ($V(CN)_3$), 11CI
Vanadium tricyanide
[82734-57-4]

$V(CN)_3$

M 128.9
Synth. from VCl_3 and NH_4CN in MeCN. Purple solid.
▷ Toxic.
Ammoniate: [82734-56-3]. *Amminetricyanovanadium*(III)
$C_3H_3N_4V$ M 146.0
Synth. by subliming $[NH_4]CN$ onto VCl_3 and then condensing NH_3 onto the mixture. Purple solid.
Paramagnetic, μ_{eff} = 2.4μ_B, Ir $\nu_{C\equiv N}$ 2120, 2095 cm^{-1}.

Dodsworth, E.S. *et al, Inorg. Chim. Acta*, 1982, **61**, 9 (*synth, uv-vis, ir, magnetism*)

$C_3N_3Zn^{\ominus}$ IC-003795

Tris(cyano)zincate(1−)
[18973-61-0]

$[Zn(CN)_3]^{\ominus}$

M 143.4 (ion)
Ph_4P salt: [73338-59-7].
Cryst.

Papp, S. *et al, Z. Anorg. Allg. Chem.*, 1979, **458**, 241 (*synth, thermal anal, ir*)

$C_3N_4NiO^{2\ominus}$ IC-003796

Tricyanonitrosylnickelate(2−), 8CI
[25703-99-5]

$[Ni(CN)_3(NO)]^{2\ominus}$

M 166.7 (ion)
Struct. unknown; may be tetrahedral. Many studies in soln. Synth. from Tetrakis(cyano-*C*)nickelate(2−), IC-004541 + NH_4OH(aq.), NH_2OH in $OH^{\ominus}$ (aq.) or NO in NH_3(l).
Di-K salt:
$C_3K_2N_4NiO$ M 244.9
Violet cryst.

Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1948, **256**, 145.
Griffith, W.P. *et al, J. Inorg. Nucl. Chem.*, 1958, **7**, 295.
Bonner, F.T. *et al, Inorg. Chem.*, 1981, **20**, 3155.

$C_3Nd_2O_9$ IC-003797

Neodymium(*III*) carbonate
[5895-46-5]

$Nd_2(CO_3)_3$

M 468.5
Red solid. Dec. >380°.
Octahydrate: [7184-63-6].
Red solid. Insol. H_2O. Loses H_2O at ~175°. 10-Coord., isostructural with La analogue. Various other hydrates also known.

[38245-38-4, 41836-16-2, 64360-95-8]

Salutsky, M.L. *et al, J. Am. Chem. Soc.*, 1950, **72**, 3306 (*synth*)
Wakita, H. *et al, Bull. Chem. Soc. Jpn.*, 1972, **45**, 2476; 1973, **46**, 152 (*synth, ir, tga, dta, struct*)
Caro, P.E. *et al, Bull. Soc. Chim. Fr.*, 1972, 46 (*struct*)
Caro, P.E. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 1167.
Firshing, F.H. *et al, J. Chem. Eng. Data*, 1986, **31**, 40 (*solv*)

$C_3NpO_{11}^{4\ominus}$ IC-003798

Tris(carbonato)dioxoneptunate(*VI*)(4−)
[57512-27-3]

$[NpO_2(CO_3)_3]^{4\ominus}$

M 449.0 (ion)
Raman ν_{NpO_2} 802 cm^{-1}.
Tetra-K salt: [19633-87-5].
Air-stable yellow-green solid (dark green cryst.). 8-Coordinate, isomorphous with U analogue. Ir ν_{NpO_2} 873 cm^{-1}.
Tetra-NH_4 salt: [36568-63-5].
Dark green solid. Dec. to $PuO_2(CO_3)$ on standing in air.
Bis[hexaaminecobalt(3+)], dinitrate double salt: [63576-32-9].
Yellow-green solid. Dec. at 150-250° ultimately to Co_3O_4 + NpO_2.

[34842-42-7, 58568-81-3, 64519-49-9]

Gorbenko-Germanov, D.S. *et al, Zh. Neorg. Khim.*, 1966, **11**, 516; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1966, **11**, 280 (*synth, struct, ir*)
Kharitonov, Yu.Ya. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1971, **200**, 613 (*ir*)
Moskvin, A.L. *et al, Radiokhimiya*, 1971, **13**, 674 (*props*)
Musikas, C. *et al, CA*, 1976, **85**, 71067 (*cryst struct*)
Saito, A. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 415; 1980, **42**, 1301 (*synth, dta, uv-vis*)
Madic, C. *et al, Inorg. Chem.*, 1983, **22**, 1494 (*raman*)
Marquart, R. *et al, J. Less-Common Met.*, 1983, **91**, 119 (*synth*)

C_3OS IC-003799

Carbon oxide sulfide (C_3OS)
3-Thioxo-1,2-propadien-1-one, 9CI. Tricarbon oxide sulfide

O=C=C=C=S

M 84.0
Interatomic distances: C=O 116.3, C=C 128.9, C=S 155.4 pm. Formed in low yield from C_3O_2 + P_4S_{10}. Mp −70°.

Winnewisser, M. *et al, Chem. Phys. Lett.*, 1976, **37**, 270 (*synth, microwave*)
Gmelin Handbook Inorg. Chem., Syst. No. 14, 1977, **D5**, 1 (*bibl*)

C_3O_2 IC-003800

Carbon oxide (C_3O_2)
1,2-Propadiene-1,3-dione, 9CI. Malonic anhydride. Tricarbon dioxide. Carbon suboxide
[504-64-3]

O=C=C=C=O

M 68.0
Interatomic distances: O=C 116.3, C=C 128.9 pm. Synth. from malonic acid and P_4O_{10}. Used in synth. of malonates. Colourless, odorous gas, polymerising above 15° to red solid. Sl. sol. CS_2, xylene. d_4^0 1.114. Mp −111.3° (−107°). Bp 7°. Burns with blue, sooty flame. In H_2O → malonic acid.
▷ Lachrymator, in high concs. attacks eyes and respiratory organs. Highly toxic.

Kobe, K.A. *et al*, *J. Phys. Chem.*, 1931, **35**, 3025 (*synth*)
Grauer, R., *Chimia*, 1960, **14**, 11 (*rev*)
Clark, A. *et al*, *Chem. Phys. Lett.*, 1970, **6**, 452 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 623 (*synth*)
Nader, F.W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1986, **25**, 93 (*synth, bibl*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 470.

IC-003801

$C_3O_9Pr_2$

Praseodymium(*III*) carbonate

[5895-45-4]

$Pr_2(CO_3)_3$

M 461.8
Formed by dehyd. of octahydrate at 60-180°. Green solid. Dec. >420°.
Trihydrate: [64360-92-5].
Loses H_2O from 220→350°.
Octahydrate: [14948-62-0].
Green solid. Insol. H_2O. μ_{eff} = 3.43μ_B. Loses H_2O >60°. 10-coordinate; isostructural with Laanalogue.
[14475-17-3, 54397-87-4]

Salutsky, M.L. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3306 (*synth*)
Sastry, R.L.N. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1165 (*synth, ir, tga, dta*)
Caro, P.E. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **267**, 1594; 1969, **269**, 687 (*synth*)
Wakita, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2476; 1973, **46**, 152 (*synth, tga, dta, ir, struct*)
Caro, P.E. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 1167 (*ir*)
Savin, V.D. *et al*, *Zh. Fiz. Khim.*, 1985, **59**, 2404 (*tga*)
Firshing, F.H., *J. Chem. Eng. Data*, 1986, **31**, 40 (*soly*)

$C_3O_9Y_2$

IC-003802

Yttrium(*III*) carbonate

[556-28-5]

$Y_2(CO_3)_3$

M 357.8
Used in synth. of Y_2O_3 etc. Colourless solid.
Dihydrate: [36833-38-2].
Colourless solid. Insol. H_2O. Compound has composition $Y_2(CO_3)_3.2.35H_2O$ as cryst. from soln.
Mineral: [12199-46-1]. ***Tengerite***
Occurs in Sweden, Japan, Quebec and Texas. White powdery cryst. Formulated as $CaY_2(CO_3)_4(OH)_2.3H_2O$.
[5970-44-5, 19512-16-4, 38245-39-5]

Head, E.L., *Inorg. Nucl. Chem. Lett.*, 1966, **2**, 33 (*synth*)
Goldsmith, J.A. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 1909 (*ir*)
Nagashima, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2476; 1973, **46**, 152 (*synth, ir, tga, dta, struct*)
Japan. Pat., 78 95 900, (1978); *CA*, **90**, 57337 (*use*)
Tareen, J.A.K. *et al*, *J. Crystal Growth*, 1980, **49**, 761 (*synth, ir, struct*)
Firshing, F.H. *et al*, *J. Chem. Eng. Data*, 1986, **31**, 40 (*soly*)

$C_3O_{11}Pu^{4\ominus}$

IC-003803

Tris(carbonato-*O*)dioxoplutonate(*VI*)(4−)

$[PuO_2(CO_3)_3]^{4\ominus}$

M 451.0 (ion)
Tetra-K salt: Green solid. Insol. H_2O.
Tetra-NH_4 salt: Dark green solid. Insol. H_2O. Dec. at 120-130° to PuO_2CO_3; also dec. on storage in air.

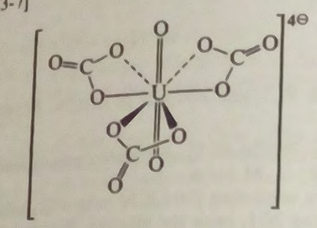
Ellinger, F.H. *et al*, *J. Phys. Chem.*, 1954, **58**, 405.
Nikol'skii, V.D. *et al*, *Radiokhimiya*, 1963, **5**, 744 (*synth*)
Keenan, T.K. *et al*, *Inorg. Chem.*, 1964, **3**, 1231.
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, C, 234 (*rev, bibl*)
Cleveland, J.M., *The Chemistry of Plutonium*, American Nuclear Society, 1979, 395 (*rev*)
Marquart, R. *et al*, *J. Less-Common Met.*, 1983, **91**, 119 (*synth*)

$C_3O_{11}U^{4\ominus}$

IC-003804

Tris(carbonato-*O*)dioxouranate(*VI*)(4−)

[24646-13-7]



M 450.0 (ion)
Hexagonal bipyramidal anion. Involved in carbonate leaching of uranium ores; potentially recoverable from oceans. Various salts are minerals.
Tetra-Na salt: [12076-52-7].
$C_3Na_4O_{11}U$ M 542.0
Unusual sol. in H_2O, rare for heavy metal carbonates, allows extraction of U from ores with conc. aq. Na_2CO_3. Light yellow triclinic cryst. Sol. H_2O. Ir ν_{OUO} 843 cm^{-1}. Raman $\nu_{(sym)OUO}$ 808 cm^{-1}.
Tetra-K salt: [17871-80-6].
$C_3K_4O_{11}U$ M 606.4
Pale yellow cryst. Isostructural with NH_4 salt. Ir ν_{OUO} 882 cm^{-1}. Raman $\nu_{(sym)OUO}$ 806 cm^{-1}.
Di-Ca salt: [64521-39-7]. ***Liebigite.*** *Urothallite*
$C_3Ca_2O_{11}U$ M 530.2
Liebigite (undecahydrate) occur as secondary mineral with widespread occurrence. Yellow-green solid (orthorhombic). Mp >160° dec. Obt. as deca- and nonahydrates. Similar compds. can be prepd. for other M(*II*) (Sr, Ba, Cu, Ni, Co).
Ca, di-Na salt: [12202-87-8]. ***Andersonite***
$C_3CaNa_2O_{11}U$ M 536.1
Andersonite (hexahydrate) occurs as secondary mineral at sites in USA and New Mexico. Yellow-green hexagonal cryst. Obt. as hexahydrate.
Ca, Mg salt: [12202-86-7]. ***Swartzite***
$C_3CaMgO_{11}U$ M 514.4
Occurs as secondary mineral at sites in USA. Bright green cryst. + $12H_2O$. Dull yellowish white (anhydrous).
Tetra-NH_4 salt: [18077-77-5]. *AUC*
$C_3H_{16}N_4O_{11}U$ M 522.2
Important in prep. of homogenous (U, Pu)O_2 fuels, and in conversion of UF_6 + $U_2(NO_3)_2$ to UO_2. Lemon-yellow or green-yellow monoclinic cryst. On heating forms U_3O_8, NH_3, CO_2. Dec. >150°.
[17872-00-3, 24764-73-6, 60897-40-7]

Berzelius, J., *Pogg. Ann. Phys. Chem.*, 1824, **1**, 359 (*synth*)
Douglas, R.M., *Anal. Chem.*, 1956, **28**, 1635 (*cryst struct*)
Apelman, D., *Geol. Soc. Am. Bull.*, 1956, **67**, 1666 (*minerals*)
Blake, C.A. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 5978 (*synth*)
Coda, A., *Rend. Soc. Mineral. Ital.*, 1963, **19**, 238 (*minerals*)
Jindra, J. *et al*, *Collect. Czech. Chem. Commun.*, 1966, **31**, 2639 (*synth*)
Hackstein, K.G. *et al*, *Atomwirtschaft.*, 1967, **12**, 524 (*use*)
Graziani, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 2059 (*cryst struct*)

Brandberg, S.G., *Nucl. Technol.*, 1973, **18**, 177 (*use*)
Bachmann, H.G. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 735 (*struct, tga*)
Ger. Pat., 2 724 710, (1977); *CA*, **90**, 139733 (*use*)
Koglin, E. *et al*, *Spectrochim. Acta, Part A*, 1979, **35**, 641 (*ir, raman, uv-vis, luminescence*)
Anderson, A. *et al*, *Can. J. Chem.*, 1980, **58**, 1651 (*synth, cryst struct, ir, raman*)
Pam, Y.M. *et al*, *J. Nucl. Med.*, 1981, **99**, 135 (*synth*)
U.S. Pat., 4 292 279, (1981); *CA*, **95**, 189468 (*manuf, use*)
Gmelin Handbook Inorg. Chem., Syst. No. 55 *Suppl. Vol.*, 1983, C13, 12 (*rev, bibl*)
Marquart, R. *et al*, *J. Less-Common Met.*, 1983, **91**, 117.
Brittain, H.G., *J. Lumin.*, 1984, **29**, 285 (*photoluminescence, uv-vis*)

C_3S_2

IC-003805

Carbon sulfide (C_3S_2)

Carbon subsulfide. Tricarbon disulfide

S=C=C=C=S

M 100.1
Formed by action of an electric discharge on CS_2. Red liq., dec. at 20° over a few weeks to a black polymer $(C_3S_2)_x$. Sol. CS_2. Mp −0.5°. Bp_{12} 60-70°.
▷ Explodes if heated rapidly to 100-120°.

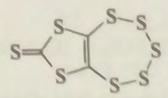
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, **1**, 653 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **22**, 107.

C_3S_8

IC-003806

[1,3]Dithiolo[4,5-*f*]-1,2,3,4,5-pentathiepin-7-thione, 9CI

[120385-42-4]



M 292.5
Struct. not certain. Yellow cryst. solid. Mass spec. indicates S_8 formula, analysis S_7. S_8 more probable.

Yang, X. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 3465 (*synth, ir, ms*)

$C_4AgN_4^{3\ominus}$

IC-003807

Tetrakis(cyano-*C*)argentate(3−), 11CI, 9CI

Tetracyanoargentate(3−), 8CI

[16743-34-3]

$[Ag(CN)_4]^{3\ominus}$ (T_d)

M 211.9 (ion)
Isomorphous with $Cu(CN)_4^{3\ominus}$.
Tri-K salt: [53833-84-4].
$C_4AgK_3N_4$ M 329.2
Colourless cryst. Sol. H_2O. Originally erroneously thought to be hydrated.

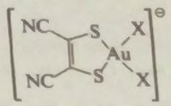
Bassett, M. *et al*, *J. Chem. Soc.*, 1924, **125**, 1660 (*synth*)
Jones, L.H. *et al*, *J. Chem. Phys.*, 1954, **22**, 965 (*ir*)
Staritzky, E. *et al*, *Anal. Chem.*, 1956, **28**, 423 (*cryst struct*)
Chantry, G.W. *et al*, *J. Chem. Phys.*, 1960, **33**, 736 (*raman*)
Nakatsuji, H. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 4653 (*Ag-109 nmr*)
Endo, K. *et al*, *J. Magn. Reson.*, 1985, **65**, 268 (*Ag-109 nmr*)
Morton, J.R. *et al*, *J. Magn. Reson.*, 1986, **67**, 211 (*esr*)

$C_4AuBr_2N_2S_2^{\ominus}$

IC-003808

(Maleonitriledithiolato)dibromoaurate(*III*)(1−)

Dibromo[2,3-dimercapto-2-butenedinitrilato(2−)-S,S']aurate(1−), 11CI



X = Br

M 496.9 (ion)
Tetrabutylammonium salt: Brown cryst. (CH_2Cl_2/Et_2O). Mp 113°.

Usón, R. *et al*, *Inorg. Chim. Acta*, 1981, **52**, 29 (*synth*)

$C_4AuCl_2N_2S_2^{\ominus}$

IC-003809

(Maleonitriledithiolato)dichloroaurate(*III*)(1−)

Dichloro[2,3-dimercapto-2-butenedinitrilato(2−)-S,S']aurate(1−), 11CI

As (Maleonitriledithiolato)dibromoaurate(*III*)(1−), IC-003808 with

X = Cl

M 408.0 (ion)
Me_4N salt: [80316-76-3].
Green cryst. (Me_2CO/Et_2O). Mp 254° dec.
[80316-78-5, 80316-80-9]

Usón, R. *et al*, *Inorg. Chim. Acta*, 1981, **52**, 29 (*synth*)

$C_4AuN_4^{\ominus}$

IC-003810

Tetrakis(cyano-*C*)aurate(1−)

Tetracyanoaurate(III)(1−)

[22806-79-7]

$[Au(CN)_4]^{\ominus}$

M 301.0 (ion)
Square planar. Interatomic distances: Au—C 199, 198, 195 pm; angles: CAuC 89.9°, 90.1°.
Na salt: [31395-95-6].
Yellow cryst. (H_2O). Sol. H_2O.
K salt: [14263-59-3].
Commercially available. Used in photographic processes and gold plating. Orthorhombic yellow cryst. + 0.5 H_2O (H_2O). Sol. H_2O. Ir ν 2189 cm^{-1}.
Ag salt: [71317-90-3].
C_4AgAuN_4 M 408.9
Insol. solid.
H compd. hydrate: From K salt by cation exchange. Stable strong acid. Monoclinic, white cryst. +$2H_2O$. Sol. H_2O. Ir ν_{CN} 2204, 2218 cm^{-1}. Formulated as $H_3O^{\oplus}Au(CN)_4^{\ominus}.H_2O$ and $H_5O_2^{\oplus}Au(CN)_4^{\ominus}$.

Smith, J.M. *et al*, *Inorg. Chem.*, 1965, **4**, 369 (*synth, ir*)
Smith, J.M. *et al*, *J. Chem. Phys.*, 1969, **41**, 2507 (*ir*)
Bertinotti, C. *et al*, *Acta Crystallogr., Sect. B*, 1970, **26**, 422 (*cryst struct*)
Penneman, R.A. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 1629 (*cryst struct*)
Japan. Pat., 78 418, (1978); *CA*, 1981, **95**, 222279 (*synth*)
Pesck, J.J. *et al*, *Inorg. Chem.*, 1979, **18**, 924 (*vmr*)

$C_4BCl_2CoO_4$ IC-003811

Tetracarbonyl(dichloroboryl)cobalt

Tetracarbonylcobaltdichloroborane

$(OC)_4CoBCl_2$

M 252.6

Brown solid. Dec. slowly on heating.

Nöth, H. *et al, Allg. Prakt. Chem.*, 1966, **17**, 610; *CA*, **66**, 25503 (*synth*)

Schmid, G., *Angew. Chem., Int. Ed. Engl.*, 1970, **9**, 819 (*rev, synth, B-11 nmr*)

$C_4BrF_9O_6S_3$ IC-003812

Bromotris(trifluoromethylsulfonyl)methane

[114395-73-2]

$CBr(SO_2CF_3)_3$

M 491.1

Synth. from $AgC(SO_2CF_3)_3$ and Br_2 in CH_2Cl_2. Subl. *in vacuo*. Mp 93.8°.

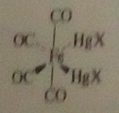
Turowsky, L. *et al, Inorg. Chem.*, 1988, **27**, 2135 (*synth, F-19 nmr, ir, ms*)

$C_4Br_2FeHg_2O_4$ IC-003813

Bis(bromomercurio)tetracarbonyliron, 8CI

Bis(bromomercury)tetracarbonyliron, 10CI

[15281-78-4]



X = Br

M 728.8

cis-form

Colourless needles or yellow solid (MeOH). Poorly sol. all solvs. Mp °*ca.*170 dec.

Hock, H. *et al, Ber. B*, 1929, **62**, 431 (*synth*)

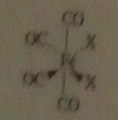
Baird, H.W. *et al, J. Organomet. Chem.*, 1967, **7**, 503 (*cryst struct*)

Bradford, C.W. *et al, J. Chem. Soc. A*, 1968, 2456 (*synth, ir, raman*)

$C_4Br_2FeO_4$ IC-003814

Dibromotetracarbonyliron(*II*), 9CI, 8CI

[18475-84-8]



X = Br

M 327.6

Octahedral

cis-form

Red-brown light-sensitive needles (pet. ether). Subl. 45–45° Dec. by H_2O.

Hieber, W. *et al, Ber.*, 1928, **61**, 1717 (*synth*)

Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1935, **190**, 193 (*ir*)

Hieber, W. *et al, Angew. Chem.*, 1956, **68**, 679 (*props*)

Taylor, R.C. *et al, Inorg. Chem.*, 1964, **3**, 584 (*synth, ir*)

Cohen, I.A. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 511 (*synth*)

Johnson, B.F.G. *et al, J. Chem. Soc. A*, 1968, 1043 (*ir*)

Butler, I.S. *et al, J. Organomet. Chem.*, 1969, **18**, 145 (*ir*)

Bancroft, G.M. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2103 (*mössbauer*)

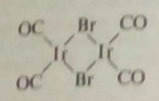
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1956 (*synth*)

Vancea, L. *et al, J. Organomet. Chem.*, 1977, **134**, 219 (*cmr*)

$C_4Br_2Ir_2O_4$ IC-003815

Di-μ-bromotetracarbonyldiiridium, 8CI

[28529-98-8]



M 656.2

Bridged dimer. Catalyst for the carboxylation of olefins.

No phys. props. reported.

Monomer: Bromodicarbonyliridium

C_2BrIrO_3 M 328.1

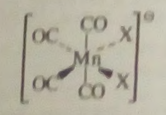
Unknown.

Ger. Pat., 1 941 501, (1970); *CA*, **72**, 110811j (*use*)

$C_4Br_2MnO_4^{\ominus}$ IC-003816

Dibromotetracarbonylmanganate(1 –)

[37176-07-1]



X = Br

M 326.7 (ion)

Et_4N salt: [43184-81-2].

Synth. from $MnBr(CO)_5$ + $[Et_4N]Br$ in diethyleneglycol dimethyl ether at 120°. Cryst.

Abel, E.W. *et al, J. Chem. Soc.*, 1964, 434 (*synth, ir, nmr*)

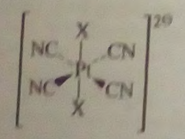
Farona, M.F. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1814 (*props*)

Connor, J.A. *et al, J. Organomet. Chem.*, 1974, **73**, 351 (*props*)

$C_4Br_2N_4Pt^{2\ominus}$ IC-003817

Dibromotetrakis(cyano)platinate(2–), 9CI

Dibromotetracyanoplatinate(IV)



X = Br

M 458.9 (ion)

trans-form [20756-58-5]

Synth. from Br_2 + $[Pt(CN)_4]^{2\ominus}$.

Di-K salt: [16922-55-7].

$C_4Br_2K_2N_4Pt$ M 537.1

Light-sensitive golden cryst. Sol. MeCN. Forms a monohydrate.

Ba salt: [64645-32-5].

$C_4BaBr_2N_4Pt$ M 596.2

Solid + $4.5H_2O$

[19585-04-7, 60118-92-5, 61374-84-3]

Mason, W.R., *Inorg. Chem.*, 1969, **8**, 1756 (*synth*)

Khartonov, Yu.Ya. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 403 (*ir*)

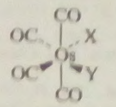
Koch, T.R. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 3249 (*cryst struct*)

Blanchard, W.D. *et al, Inorg. Chim. Acta*, 1978, **28**, 159 (*uv-vis*)

$C_4Br_2O_4Os$ IC-003818

Dibromotetracarbonylosmium, 9CI, 8CI

[14878-21-8]



cis-form

X = Y = Br

M 462.0

Earlier work reports both a colourless and a yellow form. Later work only reports a colourless *cis*-form.

cis-form [18953-16-7]

Synth. from $OsH_2(CO)_4$ and CBr_4 in heptane. Colourless solid. Mp 317° dec.

Yellow-form

May be *trans*-form.

Hieber, W. *et al, Chem. Ber.*, 1942, **75**, 1472 (*synth*)

L'Eplattenier, F. *et al, Inorg. Chem.*, 1967, **6**, 2092 (*synth, ir*)

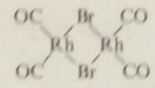
Hales, L.A.W. *et al, J. Chem. Soc. A*, 1967, 1389, 1932 (*synth, ir*)

$C_4Br_2O_4Rh_2$ IC-003819

Di-μ-bromotetracarbonyldirhodium, 10CI

Tetracarbonyldi-μ-bromodirhodium

[21475-96-7]



M 477.6

Bridged dimer. Red cryst. (hexane). Mp 118°. Ir ν_{CO} 2040s, 2090s, 2115w cm^{-1} (nujol).

Monomer: Bromodicarbonylrhodium. Dicarbonylrhodium bromide

C_2BrO_2Rh M 238.8

Unknown.

Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1943, **251**, 98 (*synth*)

Garland, C.W. *et al, J. Chem. Phys.*, 1962, **36**, 1094 (*ir*)

Lewis, J. *et al, Acc. Chem. Res.*, 1968, **1**, 245 (*ms*)

Colton, R. *et al, Aust. J. Chem.*, 1970, **23**, 1351 (*ir, synth*)

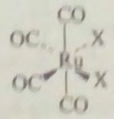
Brown, C. *et al, J. Organomet. Chem.*, 1980, **192**, 93 (*nmr, synth*)

Nixon, J.F. *et al, Inorg. Chim. Acta*, 1981, **47**, 147 (*synth, pe*)

$C_4Br_2O_4Ru$ IC-003820

Dibromotetracarbonylruthenium, 9CI, 8CI

[15663-29-3]



X = Br

M 372.9

cis-form [21439-16-7]

Yellow cryst.

Calderazzo, F. *et al, Inorg. Chem.*, 1967, **6**, 1220 (*synth*)

Cotton, J.D. *et al, J. Chem. Soc. A*, 1968, 2162 (*synth*)

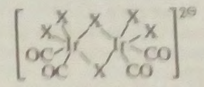
Johnson, B.F.G. *et al, J. Chem. Soc. A*, 1969, 792 (*synth, ir*)

Benedetti, E. *et al, J. Organomet. Chem.*, 1972, **37**, 361 (*synth, ir*)

$C_4Br_6Ir_2O_4^{2\ominus}$ IC-003821

Di-μ-bromotetrabromotetracarbonyldiiridate(2–), 8CI

Hexabromotetracarbonyldiiridate(2–)



X = Br

M 975.9 (ion)

Bis-Ph_4As salt: [31390-54-2].

Yellow cryst. (Me_2CO/pet. ether). Ir ν_{CO} 2090, 2057 cm^{-1} (Me_2CO).

Clears, M.J. *et al, J. Chem. Soc. A*, 1970, 2788 (*synth, ir, struct*)

$C_4CaMg_2O_{12}$ IC-003822

Calcium magnesium carbonate ($CaMg_2(CO_3)_4$)

Carbonic acid, calcium magnesium salt (4:1:3), 8CI

Calcium magnesium carbonate $CaMg_2(CO_3)_4$

[22450-53-9]

$CaMg_2(CO_3)_4$

M 353.0

Isotypic with calcite; Ca and Mg are ordered in the same cation plane with Ca in trigonal prismatic and Mg in edge-sharing O_6 sites. Manuf. from the ore by traditional extraction methods. White powder. Dec. on heating with CO_2 loss to form MgO and CaO. Prac. insol. H_2O. ΔH_f° –4530 kJ mol^{-1}; ΔG_f° –4204 kJ mol^{-1}.

Mineral-form [19569-21-2]

Huntite

Isostructural with Daquigshanite. Widespread occurrence as a cave-carbonate. White, earthy, fibrous mass.

Graf, D.L. *et al, Acta Crystallogr.*, 1962, **15**, 238 (*cryst struct*)

Hemingway, B.S. *et al, J. Res. U.S. Geol. Surv.*, 1973, **1**, 535 (*thermochem data*)

Schott, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **280**, 1247 (*thermochem data*)

Scheetz, B.E. *et al, Am. Mineral.*, 1977, **62**, 36 (*ir, raman*)

Ozao, R. *et al, Thermochim. Acta*, 1985, **86**, 45 (*thermal dec*)

Dollase, W.A. *et al, Am. Mineral.*, 1986, **71**, 163 (*cryst struct*)

$C_4CdF_6O_4$ IC-003823

Bis(trifluoroacetato-*O*)cadmium

Cadmium trifluoroacetate

[37054-04-9]

$Cd(OOCCF_3)_2$

M 338.4

Cryst. Insol. hexane.

Kalinina, G.S. *et al, J. Gen. Chem. USSR* (*Engl. Transl.*), 1972, **42**, 144 (*synth*)

$C_4CdN_4^{2\ominus}$ IC-003824

Tetrakis(cyano-*C*)cadmate(2–)

Tetracyanocadmate(2–)

[16041-14-8]

$[Cd(CN)_4]^{2\ominus}$

M 216.4 (ion)

Di-K salt: [14402-75-6].

$C_4CdK_2N_4$ M 294.6

Cryst.

Di-Cs salt: [15634-22-7].

$C_4CdCs_2N_4$ M 482.2
Cryst.
Bis(1,2-ethanediamine-N,N′)cadmium(2+) salt: [98255-12-0].

$C_8H_{16}Cd_2N_8$ M 449.0
Acts as a chelate host for such guests as C_6H_6.
Bis(1,2-ethanediamine-N,N′)cadmium(2+) salt, bis-C_6H_6 clathrate: [98255-13-1].

$C_{20}H_{28}Cd_2N_8$ M 605.3
Clathrate compd., contains bridging ethylenediamine groups.
Bis(diphenyliodonium) salt: [73012-27-8].

$C_{28}H_{28}CdI_2N_4$ M 778.7
Cryst.
[37286-73-0]

Bok, L.D.L. *et al, J. S. Afr. Chem. Inst.*, 1966, **19**, 62 (*synth, powder struct, Cs salt*)
Kalani, D.K. *et al, Lab. Pract.*, 1969, **18**, 275 (*ir*)
Ikeda, R., *Nippon Kagaku Zasshi (Jpn. J. Chem.)*, 1969, **90**, 721 (*nqr*)
Persson, H., *Acta Chem. Scand.*, 1971, **25**, 343 (*stability const*)
Dehnicke, G. *et al, Ber. Bunsenges. Phys. Chem.*, 1974, **78**, 1010 (*ir, K salt*)
Ohyama, J. *et al, Bull. Chem. Soc. Jpn.*, 1977, **50**, 410 (*synth, powder struct, $Cd(en)_3$ salt*)
Schmidt, K.H., *Spectrochim. Acta, Part A*, 1977, **33**, 369 (*ir, raman, K salt*)
Iwamoto, T. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 488 (*clathrates*)
Pasek, J.J. *et al, Inorg. Chem.*, 1979, **18**, 924 (*cmr, ion*)
Gyoryova, K. *et al, Acta Chim. Acad. Sci. Hung.*, 1981, **107**, 167 (*thermal dec, Ph_4J salt*)
Sano, M. *et al, Inorg. Chem.*, 1982, **21**, 2521 (*cmr, N-15 nmr, ion*)
Wasylishen, R.E. *et al, J. Mol. Struct.*, 1982, **79**, 415 (*raman, phase trans, K salt*)
Gyoryova, K., *Chem. Zvesti*, 1983, **37**, 773 (*synth, ir, Ph_4J salt*)
Nishikiori, S. *et al, J. Inclusion Phenom.*, 1985, **3**, 283 (*synth, cryst struct, clathrate formn, $Cd(en)_3$ salt*)

$C_4CdN_4O_4^{2\ominus}$ IC-003825
Tetrakis(fulminato-*C*)cadmate(2−)
[45068-17-5]

$[Cd(CNO)_4]^{2\ominus}$

M 280.4 (ion)
Bis-tetrapropylammonium salt: [30179-36-3].
Colourless cryst. (EtOH/Et_2O). Sol. Me_2CO, CH_2Cl_2, EtOH, H_2O; insol. Et_2O, pet. ether. Mp 118°.
Bis-Ph_4As salt: [30179-37-4].
Colourless cryst. Mp 231°.

Beck, W. *et al, Chem. Ber.*, 1970, **103**, 3591 (*synth, ir*)
Beck, W. *et al, Z. Naturforsch., B*, 1973, **28**, 229 (*ir, raman*)

$C_4CdN_4S_4^{2\ominus}$ IC-003826
Tetrakis(thiocyanato)cadmate(2−)
[16041-16-0]

$[Cd(NCS)_4]^{2\ominus}$

M 344.7 (ion)
Both Cd—NCS and Cd—SCN connections have been detected in soln.; in H_2O 2NCS are bonded to Cd via *S* and 2 via *N*. In DMF and in DMSO only 1 Cd—SCN group.
Di-Na salt: Solid + $2H_2O$.
Di-K salt: [15006-40-3].
Solid + $2H_2O$ (H_2O).
Mg salt: Solid + $2H_2O$.
Ca salt: Solid + $3H_2O$.
Bis-Me_4N salt: [110591-67-8].
Cryst. (Me_2CO). Polymeric anion with 6-coord. Cd and 4 bridging NCS groups per Cd.
Bis-Et_4N salt: [70713-96-1].
Cryst.
Bis-tetrabutylammonium salt: [73293-38-6].
Cryst.
(Diethylenetriamine)cadmium(2+) salt: see *Bis(diethylenetriamine)tetrakis(thiocyanato)dicadmium, IC-007902*
[45068-20-0, 121777-95-5]

Taylor, K.A. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1967, **47**, 138 (*raman of ion*)
Gerding, P., *Acta Chem. Scand.*, 1968, **22**, 1283 (*stability const*)
Kharitonov, Yu.Ya. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 364 (*ir*)
Tsivadze, A.-Yu. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1094 (*synth, ir*)
Kargol, J.A. *et al, Inorg. Chem.*, 1979, **18**, 2532 (*cmr, Et_4N salt*)
Pregosin, P.S. *et al, Inorg. Chim. Acta*, 1980, **38**, 237 (*N-15 nmr, Bu_4N salt*)
Anti-Jovanovic, A. *et al, J. Raman Spectrosc.*, 1982, **12**, 91 (*raman*)
Yamaguchi, T. *et al, Bull. Chem. Soc. Jpn.*, 1985, **58**, 3235 (*pe, raman, cmr, N-14 nmr*)
Oldham, C. *et al, Inorg. Chim. Acta*, 1985, **100**, L9 (*synth*)
Kuniyasu, Y. *et al, Bull. Chem. Soc. Jpn.*, 1987, **60**, 179 (*synth, cryst struct, ir*)
Ohtaki, H., *Pure Appl. Chem.*, 1987, **59**, 1143 (*soln struct*)
Ishiguro, S.-I. *et al, Bull. Chem. Soc. Jpn.*, 1988, **61**, 3901 (*raman*)

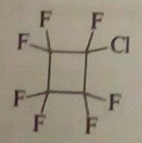
$C_4CdN_4Se_4^{2\ominus}$ IC-003827
Tetrakis(selenocyanato-*N*)cadmate(2−)
Tetraisoselenocyanatocadmate(2−)
[17967-96-3]

$[Cd(NCSe)_4]^{2\ominus}$

M 532.3 (ion)
Di-K salt: [26024-28-2].
$C_4CdK_2N_4Se_4$ M 610.5
Cryst.
Bis-Ph_4As salt: [41898-59-3].
Cryst.

Alasaniya, R.M. *et al, Tr. -Gruz. Politekh. Inst. im. V.I. Lenina*, 1968, 28 (*ir, synth, K salt*)
Joergensen, C.K. *et al, Kgl. Dan. Vidensk. Selsk. Mata.-Fys. Medd.*, 1972, 38 (*pe, Ph_4As salt*)
Singh, P.P. *et al, J. Coord. Chem.*, 1979, **9**, 65.

C_4ClF_7 IC-003828
1-Chloro-1,2,2,3,3,4,4-heptafluorocyclobutane
Fluorocarbon C-317
[377-41-3]



M 216.4
Refrigerant. Electrical insulating liquid. d_4^{15} 1.602. Mp −39.1°. Bp 23-25° (25.6°).

Edgell, W.F., *J. Am. Chem. Soc.*, 1947, **69**, 660 (*ir, raman*)
U.S. Pat., 2 427 116, (1947); *CA*, **42**, 594c (*synth*)

$C_4ClF_9O_6S_3$ IC-003829
Chlorotris(trifluoromethylsulfonyl)methane
[114395-72-1]

$CCl(SO_2CF_3)_3$

M 446.6
Synth. from $AgC(SO_2CF_3)_3$ and Cl_2 in CH_2Cl_2. Colourless cryst., subl. *in vacuo*. Mp 69.1°.

Turowsky, L. *et al, Inorg. Chem.*, 1988, **27**, 2135 (*synth, ir, ms, F-19 nmr*)

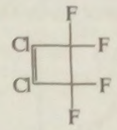
$C_4ClNO_9Ru^{2\ominus}$ IC-003830
Chloro(nitrosyl)bis(oxalato)ruthenate(2−)
Chlorobis(ethanedioato-O,O′)(nitrosyl)ruthenate(2−)

$[Ru(NO)Cl(C_2O_4)_2]^{2\ominus}$

M 342.5 (ion)
Isomeric form unknown.
Di-K salt: Prepd. by treating $K_2[Ru(NO)Cl_5]$ with $K_2[C_2O_4]$.

Charonnat, R., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1924, **178**, 1423 (*synth*)
Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 188 (*synth*)

$C_4Cl_2F_4$ IC-003831
1,2-Dichloro-3,3,4,4-tetrafluorocyclobutene, 9CI
Fluorocarbon C-1314
[377-93-5]



M 194.9
d_4^{25} 1.534. Mp −43.4° (−48°). Bp 67.1°. n_D^{25} 1.3699.

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1947, **69**, 281 (*synth, props*)
Harris, R.K. *et al, J. Magn. Reson.*, 1969, **1**, 362 (*F-19 nmr*)
King, B.R. *et al, J. Fluorine Chem.*, 1972, **1**, 283 (*synth*)
Chia, L.S. *et al, Can. J. Chem.*, 1974, **52**, 3484 (*Cl-nqr*)
Bauer, G. *et al, Z. Naturforsch., B*, 1979, **34**, 1249 (*synth*)

$C_4Cl_2F_6$ IC-003832
1,2-Dichloro-1,2,3,3,4,4-hexafluorocyclobutane
C-316
[356-18-3]

M 232.9
Synth. by cyclodimerisation of CF_2=CFCl. Liq. d_{17} 1.644. Mp −15.1°. Bp 59.9°.
▷ GU1760000.

Henne, A.L. *et al, J. Am. Chem. Soc.*, 1947, **69**, 279 (*synth*)
Miller, W.T., *Prep. Prop. Tech. Fluorinene and Organic Fluoro Compounds*, McGraw-Hill, NY, 1951, 567, 592.

$C_4Cl_2FeHg_2O_4$ IC-003833
Tetracarbonylbis(chloromercury)iron, 9CI
[15281-84-2]
As Bis(bromomercurio)tetracarbonyliron, IC-003813 with X = Cl

M 639.9
cis-form
Pale-yellow solid (Me_2CO). V. spar. sol. most org. solvs., sol. DMSO. Mp 155-160° dec.

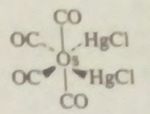
Hock, H. *et al, Chem. Ber.*, 1928, **61**, 2097; 1929, **62**, 2690 (*synth*)
Lewis, J. *et al, J. Chem. Soc. A*, 1966, **69** (*synth, ir*)
Raston, C.L. *et al, Aust. J. Chem.*, 1976, **29**, 1905 (*cryst struct*)

$C_4Cl_2FeO_4$ IC-003834
Tetracarbonyldichloroiron(*II*), 9CI, 8CI
[21475-90-1]
As Dibromotetracarbonyliron(*II*), IC-003814 with X = Cl

M 238.7
Octahedral.
cis-form
V. unstable, light-sensitive yellow powder. Dec. on attempted subl.

Hieber, W. *et al, Ber., B*, 1928, **61**, 1717 (*synth*)
Noack, K., *Helv. Chim. Acta*, 1962, **45**, 1847 (*ir*)
Taylor, R.C. *et al, Inorg. Chem.*, 1964, **3**, 584 (*synth, ir*)
Bennett, M.A. *et al, J. Chem. Soc.*, 1964, 5560 (*synth*)
Lewis, J. *et al, Acc. Chem. Res.*, 1968, **1**, 245 (*ms*)
Bancroft, G.M. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2163 (*mössbauer*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1956 (*synth*)

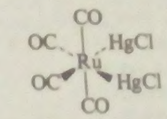
$C_4Cl_2Hg_2O_4Os$ IC-003835
Tetracarbonylbis(chloromercurio)osmium, 8CI
[21710-55-4]



M 774.3
White solid. Mp *ca.* 235° dec.

Bradford, C.W. *et al, J. Chem. Soc. A*, 1968, 2456 (*synth, ir, raman*)

$C_4Cl_2Hg_2O_4Ru$ IC-003836
Tetracarbonylbis(chloromercurio)ruthenium, 8CI



M 685.1
cis-form [21710-53-2]
Pale-yellow solid. Mp 170-175° dec.

Bradford, C.W. *et al, J. Chem. Soc. A*, 1968, 2456 (*synth, ir*)

$C_4Cl_2MnO_4^{\ominus}$ IC-003837
Tetracarbonyldichloromanganate(1−)
As Dibromotetracarbonylmanganate(1−), IC-003816 with X = Cl

M 237.8 (ion)
Et_4N salt: [52901-72-1].

Synth. from $MnCl(CO)_5$ and $[Et_4N]Cl$ in diethyleneglycol dimethyl ether at 120°. Cryst.

Abel, E.W. *et al*, *J. Chem. Soc.*, 1964, 434 (*synth, ir, nmr*)
Farona, M.F. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1814 (*props*)
Connor, J.A. *et al*, *J. Organomet. Chem.*, 1974, **73**, 351 (*props*)

$C_4Cl_2N_4Ni^{2\ominus}$ IC-003838

Dichlorotetrakis(cyano-*C*)nickelate(5−), 9Cl

Dichlorotetracyanonickelate(I)(5−)

[50507-57-8]

$[NiCl_2(CN)_4]^{5\ominus}$

M 233.6 (ion)

Octahedral, both *cis* and *trans* isomers identified. Formed on irradiation of K salt of Tetrakis(cyano-*C*)nickelate(2−), IC-004541 doped in KCl lattices.

[54003-02-0, 59461-47-1]

Jain, S.C. *et al*, *J. Chem. Phys.*, 1975, **62**, 4366.
Zanette, S.I. *et al*, *J. Chem. Phys.*, 1976, **64**, 3381.

$C_4Cl_2N_4Ni^{3\ominus}$ IC-003839

Dichlorotetrakis(cyano-*C*)nickelate(3−), 9Cl

Dichlorotetracyanonickelate(III)(3−)

[50381-46-9]

$[NiCl_2(CN)_4]^{3\ominus}$

M 233.6 (ion)

Octahedral, both *cis* and *trans* isomers identified. Formed on irradiation of K salt of Tetrakis(cyano-*C*)nickelate(2−), IC-004541 doped into KCl solid, or by addition of chloride ion to electrochemically oxidised aq. K salt of Tetrakis(cyano-*C*)nickelate(2−), IC-004541.

[54003-01-9, 59461-46-0]

Jain, S.C. *et al*, *J. Chem. Phys.*, 1975, **62**, 4366.
Zanette, S.I. *et al*, *J. Chem. Phys.*, 1976, **64**, 3381.
Pappeninagen, T.L. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 4576.

$C_4Cl_2N_4Pt^{2\ominus}$ IC-003840

Dichlorotetrakis(cyano-*C*)platinate(2−), 9Cl

Dichlorotetracyanoplatinate(IV)

As Dibromotetrakis(cyano)platinate(2−), IC-003817 with

X = Cl

M 370.0 (ion)

trans-form [20756-57-4]
Synth. from Cl_2 + $[Pt(CN)_4]^{2\ominus}$.

Di-K salt: [16924-77-9].
$C_4Cl_2K_2N_4Pt$ M 448.2
Yellow solid. Sol. MeCN.

Bis-Et_4N salt: [67572-99-0].
Sol. MeCN.

[12072-77-4, 19585-03-6, 38725-65-4]

Kharitonov, Yu.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 403 (*ir*)
Mason, W.R., *Inorg. Chem.*, 1970, **9**, 1528 (*synth*)
Blanchard, W.D. *et al*, *Inorg. Chim. Acta*, 1978, **28**, 159 (*uv-vis*)

$C_4Cl_2O_4Os$ IC-003841

Tetracarbonyldichloroosmium, 9Cl

Dichlorotetracarbonylosmium

[22873-63-8]

As Dibromotetracarbonylosmium, IC-003818 with

X = Y = Cl

M 373.1

trans-form [42230-39-7]
Colourless cryst. (CH_2Cl_2). Mp 300° dec.

cis-form [19052-51-8]
Synth. from $OsH_2(CO)_4$ and CCl_4 in C_6H_6 or $OsCl_3$ with CO at 65 atm. and 55°. Colourless cryst. ($CHCl_3$). Spar. sol. org. solvs. Ir 2187 w, 2119 vs, 2092 s, 2051 s cm^{-1}.

L'Eplattenier, F. *et al*, *Inorg. Chem.*, 1967, **6**, 2092 (*synth, ir*)
Collman, J.P. *et al*, *Inorg. Chem.*, 1974, **13**, 1 (*synth, ir*)
Tyler, D.R. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 3022 (*synth*)
Psaro, R. *et al*, *Inorg. Chim. Acta*, 1983, **77**, L255 (*synth*)
Zanoni, R. *et al*, *J. Mol. Struct.*, 1985, **131**, 363 (*pe*)

$C_4Cl_2O_4Ru$ IC-003842

Tetracarbonyldichlororuthenium, 8Cl

As Dibromotetracarbonylruthenium, IC-003820 with

X = Cl

M 284.0

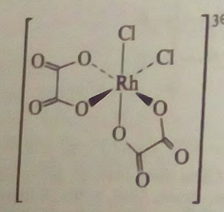
cis-form [21475-91-2]
Yellow.

Allegra, G. *et al*, *Tetrahedron Lett.*, 1965, 4187 (*synth*)
Johnson, B.F.G. *et al*, *J. Chem. Soc. A*, 1969, 792 (*synth, ir*)
Bruce, M.I. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 1325 (*synth, ir*)

$C_4Cl_2O_8Rh^{3\ominus}$ IC-003843

Dichlorodioxalatorhodate(*III*)(3−)

Dichlorobis[ethanedioato(2−)-O,O′]rhodate(III)(3−), *9Cl*



cis-form

M 349.8 (ion)

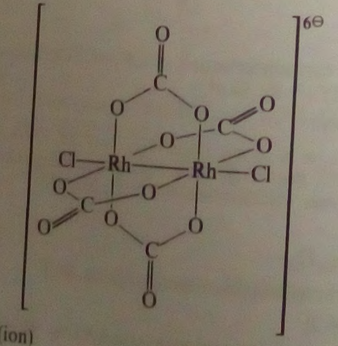
cis-form
Tri-K salt: Yellow cryst. + $3H_2O$.

trans-form
Tri-K salt: Yellow-orange cryst. + xH_2O.

Jorgensen, C.K., *Acta Chem. Scand.*, 1957, **11**, 151 (*uv*)
Gillard, R.D. *et al*, *J. Chem. Soc.*, 1964, 870 (*synth, ir*)

$C_4Cl_2O_{12}Rh_2^{6\ominus}$ IC-003844

Tetrakis[μ-carbonato(2−)-*O:O′*]dichlorodirhodate(*II*)(6−), 10Cl



M 516.7 (ion)

Tetra-Cs, di-Na salt: [63179-41-9].
Green cryst.

Cotton, F.A. *et al*, *Inorg. Chem.*, 1980, **19**, 320 (*synth, cryst struct*)

$C_4Cl_3FeO_4P$ IC-003845

Tetracarbonyl(phosphorous trichloride)iron, 8Cl

[16388-48-0]

$Cl_3PFe(CO)_4$

M 305.2
Characterised spectroscopically.

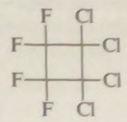
Tripathi, J.B.P. *et al*, *J. Organomet. Chem.*, 1967, **9**, 307 (*synth, ir*)

$C_4Cl_4F_4$ IC-003846

1,1,2,2-Tetrachloro-3,3,4,4-tetrafluorocyclobutane, 9Cl

Fluorocarbon C-314

[336-50-5]



M 265.8
Synth. by cyclodimerisation of $CF_2{=}CCl_2$. Solv. for C_2ClF_3 polymers. Reference compd. for F-19 nmr. Fp 81° (84.8°). Bp 131° (131.6°).

Henne, A.L. *et al*, *J. Am. Chem. Soc.*, 1947, **69**, 279 (*synth, ir*)
Harris, R.K. *et al*, *J. Magn. Reson.*, 1969, **1**, 362 (*F-19 nmr*)
Harris, W.C. *et al*, *J. Mol. Struct.*, 1973, **18**, 257 (*ir*)
Park, J.D. *et al*, *J. Org. Chem.*, 1973, **38**, 4026 (*synth*)
Hawkes, G.E. *et al*, *J. Org. Chem.*, 1974, **39**, 1276 (*cmr*)
Chew, S. *et al*, *Thermochim. Acta*, 1976, **16**, 121 (*props*)
Brabets, R. *et al*, *J. Fluorine Chem.*, 1988, **41**, 311 (*props*)

$C_4Cl_4Ir_2O_4^{\ominus}$ IC-003847

Tetracarbonyltetrachlorodiiridate(1−), 10Cl

Tetrachlorotetracarbonyldiiridate(1−)

$[Ir_2(CO)_4Cl_4]^{\ominus}$

M 638.2 (ion)
Solid contains conducting linear chains of *cis*-$Ir(CO)Cl_2^{0.6\ominus}$ units.

K salt: [12703-90-1].
$C_4Cl_4Ir_2KO_4$ M 677.3
Golden hair-like needles.

Benzyltrimethylammonium salt: Brown cryst. (MeOH).

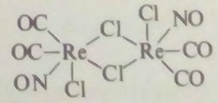
Ph_4As salt: Brown needles. Insol. all solvs. Mp 225° dec.

Malatesta, L. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **19**, 81 (*synth*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1970, 2788 (*synth, ir*)
Ginsberg, A.P. *et al*, *Inorg. Chem.*, 1976, **15**, 514 (*synth, ir, mössbauer, struct*)
Kaplunov, M.G. *et al*, *Koord. Khim.*, 1976, **2**, 1268 (*pe, ir*)

$C_4Cl_4N_2O_6Re_2$ IC-003848

Tetracarbonyldi-μ-chlorodichlorodinitrosyldirhenium, 9Cl

[25360-92-3]



M 686.2

Synth. from $[Re(CO)_4Cl]_2$ or $Re_2(NO)(CO)_5Cl_3$, NO and HCl. Starting material for rhenium nitrosyl chemistry. Stable yellow cryst. (CH_2Cl_2/hexane, CCl_4/heptane), dec. at 268°. Sol. Me_2CO, C_6H_6, $PhNO_2$, chlorinated hydrocarbons; insol. aliphatic hydrocarbons. $Subl._{0.5\,mm}$ 110°. Ir ν_{CO} 2106vs, 2047vs, ν_{NO} 1803vs cm^{-1} (CCl_4).

Monomer: Dicarbonyldichloronitrosylrhenium
$C_2Cl_2NO_3Re$ M 343.1
Unknown.

Zingales, F. *et al*, *Inorg. Chem.*, 1971, **10**, 507 (*synth, ir*)
Norton, J.R. *et al*, *Inorg. Chem.*, 1973, **12**, 485 (*synth, props, ms*)
Inorg. Synth., 1976, **16**, 35 (*synth, ir, ms*)

$C_4Cl_4N_4Se_2V$ IC-003849

Tetrachlorobis(monoselenium dicyanide-*Se*)vanadium(*IV*), 11Cl

Vanadium(IV) *chloride bis(selenium dicyanide)*

[85041-24-3]

$VCl_4[Se(CN)_2]_2$

M 454.7
trans-Octahedral. Synth. from VCl_4 and $Se(CN)_2$ in CS_2. Yellow, readily hydrol. solid. V. sol. Me_2CO. Mp 196° dec. Paramagnetic, $g_{\parallel}$ 1.954, $g_{\perp}$ 1.983.

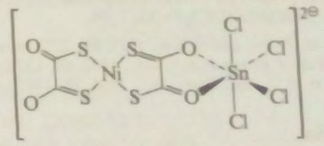
▷ $Se(CN)_2$ is probably toxic and hydrol. may yield HCN.

Delgado, M.S. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **493**, 187 (*synth, ir, esr*)

$C_4Cl_4NiO_4S_4Sn^{2\ominus}$ IC-003850

Tetrachlorobis(1,2-dithiooxalato)stannatenickelate(*II*)(2−), 8Cl

Bis[ethanebis(thioato)(2−)](tetrachlorostannate)nickelate(II)(2−)



M 559.5 (ion)
Square planar Ni, octahedral Sn. Synth. from Bis(dithiooxalato)nickelate(*II*)(2−), IC-004576 + $SnCl_4$. Corresp. compds. known for Br, I.

Bis(benzyltriphenylphosphonium) salt: [26342-84-7].
Blue cryst. (CH_2Cl_2/Et_2O). Mp 163-164°, Mp 204°.

Coucouvanis, D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 3875 (*synth, cryst struct, ir, uv, electrochem*)
Bowmaker, G.A. *et al*, *Inorg. Chem.*, 1982, **21**, 3565 (*electrochem*)

$C_4Cl_5Ir_2O_4^{2\ominus}$ IC-003851

Tetracarbonylpentachlorodiiridate(2−), 9Cl

$Ir_2(CO)_4Cl_5^{2\ominus}$

M 673.7 (ion)

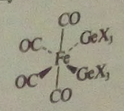
Di-K salt: [12703-91-2].
Hair-like cryst. with golden lustre (Me_2CO). Cryst. contain conducting linear chains of *cis*-$Ir(CO)_2Cl_2^{0.6\ominus}$ units with interstitial KCl.

Bis-Ph_4As salt: Golden-brown powder.

Malatesta, L. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **19**, 81 (*synth*)
Ginsberg, A.P. *et al*, *Inorg. Chem.*, 1976, **15**, 514 (*synth, ir, mössbauer, struct*)
Kaplunov, M.G. *et al*, *Koord. Khim.*, 1976, **2**, 1268 (*ir, pe*)

$C_4Cl_6FeGe_2O_4$

Tetracarbonylbis(trichlorogermyl)iron, 8CI



cis-form

X = Cl

M 525.8

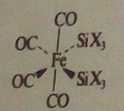
cis-form [19601-38-8]
More stable isomer. Yellow cryst. Sol. nonpolar solvs. $Subl._{0.02}$ 40-50° (part dec.). Readily hydrol. by moist air.

trans-form [19601-39-9]
White cryst. or large v. pale yellow octahedral cryst. Spar. sol. nonpolar solvs. Isom. rapidly in soln. to *cis*-form. Readily hydrol. by moist air.

Kummer, R. *et al*, *Inorg. Chem.*, 1968, **7**, 1208 (*synth, ir*)

$C_4Cl_6FeO_4Si_2$

Tetracarbonylbis(trichlorosilyl)iron, 8CI



cis-form

X = Cl

M 436.7

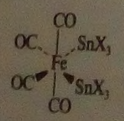
cis-form [29660-80-8]
Yellow cryst. (hexane at −80°). Mp 94-96°.

trans-form [19632-60-1]
No phys. props. recorded. Compound reported as *trans*-form is probably $(OC)_4Fe(SiCl_3)H$.

Jetz, W. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2773 (*synth, ir*)
Kahn, O. *et al*, *J. Organomet. Chem.*, 1967, **10**, 137 (*synth, ir*)
Vancea, L. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1407 (*cmr*)

$C_4Cl_6FeO_4Sn_2$

Tetracarbonylbis(trichlorostannyl)iron, 9CI



cis-form

X = Cl

M 618.0

cis-form [19601-41-3]
Yellow-orange cryst. (pentane at −80°). Readily hydrol. by moist air.

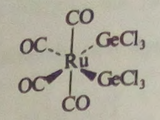
trans-form [19601-42-4]
Large yellow cryst. (pet. ether). V. sol. CH_2Cl_2, cyclohexane. Isom. to *cis*-form after 1 hr. in CH_2Cl_2. Readily hydrol. by moist air.

Kummer, R. *et al*, *Inorg. Chem.*, 1968, **7**, 1208 (*synth*)
Pomeroy, R.K. *et al*, *Inorg. Chem.*, 1977, **16**, 1508 (*nmr, stereochem*)

$C_4Cl_6Ge_2O_4Ru$

Tetracarbonylbis(trichlorogermyl)ruthenium, 9CI

[37834-28-9]



M 571.0

cis-form [34397-63-2]
White cryst. (CH_2Cl_2/hexane). Mp 90-100° dec.

Knox, S.A.R. *et al*, *J. Chem. Soc. A*, 1971, 2874 (*synth, ir*)
Ball, R. *et al*, *Inorg. Chem.*, 1972, **11**, 1806 (*cryst struct*)
Vancea, L. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1407 (*cmr*)

$C_4Cl_6Ir_2O_4^{2\ominus}$

Tetracarbonyldi-μ-chlorotetrachlorodiiridate(2−), 9CI

Tetracarbonylhexachlorodiiridate(2−)

As Di-μ-bromotetrabromotetracarbonyldiiridate(2−), IC-003821 with

X = Cl

M 709.1 (ion)

Bis-Ph₄As salt: [31471-23-5].
$C_{52}H_{40}As_2Cl_6Ir_2O_4$ M 1475.8
Yellow cryst. (Me_2CO/pet. ether). Ir ν_{CO} 2092, 2051 cm^{-1} (Me_2CO).

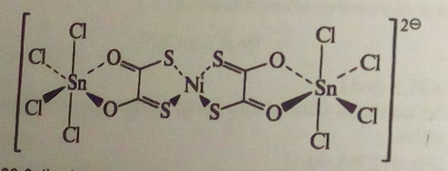
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1970, 2788 (*synth, ir, struct*)
Ginsberg, A.P. *et al*, *Phys. Lett.*, 1976, **38**, 310 (*mössbauer*)

$C_4Cl_8NiO_4S_4Sn_2^{2\ominus}$

Octachlorobis[μ-(1,2-dithiooxalato)]distannatenickelate(*II*)(2−), 8CI

Bis[μ-[ethanebis(thioato)(2−)-O,O′:S,S′]]bis(tetrachlorostannate)nickelate(II)(2−), *9CI*

[60240-65-5]



M 820.0 (ion)
Square planar Ni, octahedral Sn. Synth. from Bis(dithiooxalato)nickelate(*II*)(2−), IC-004576 + $SnCl_4$. Electrochem. studies show redox processes on ligand, not found if $SnCl_4$ units absent. Corresp. Br, I complexes also known.

Bis(benzyltriphenylphosphonium) salt: [26342-83-6].
Blue cryst. (CH_2Cl_2/Et_2O). Mp 219-220°.

[43068-61-7]

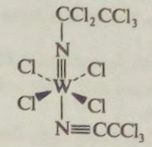
Coucouvanis, D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 3875 (*synth, cryst struct, ir, uv, electrochem*)
Bowmaker, G.A. *et al*, *Inorg. Chem.*, 1982, **21**, 3565 (*electrochem*)

$C_4Cl_{12}N_2W$

Tetrachloro(pentachloroethylimido)(trichloroacetonitrile)tungsten(*VI*)

Hexachlorobis(trichloroacetonitrile)tungsten, 8CI (incorr.).
Tetrachloro[1,1,2,2-pentachloroethanaminato(2−)](trichloroacetonitrile)tungsten, 9CI

[34822-24-7]



M 685.3
Initially postulated as $WCl_6.2Cl_3CCN$ but cryst. struct. showed chlorination of Cl_3CCN had occurred, with formation of a W≡N bond. Interatomic distances: W≡N 170, W—N 237 pm. Synth. from WCl_6 refluxed with excess Cl_3CCN in sealed ampoule. Yellow cryst. (CH_2Cl_2), non-conducting in $MeNO_2$. Many similar compds. of formula $[WCl_4(NCRCl_2)]$.RCN are known, Ir ν_{CN} 2300, $\nu_{W\equiv N}$ 1296, 1288 cm^{-1}.

[28302-55-8, 64727-94-2]

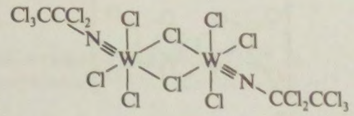
Fowles, G.W.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 459.
Drew, M.G.B. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 1219 (*cryst struct, ir*)
Fowles, G.W.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1871; 1977, 1212, 2128 (*reactions, ir, nmr*)

$C_4Cl_{18}N_2W_2$

Di-μ-chlorohexachlorobis(pentachloroethylimido)ditungsten(*VI*)

Di-μ-chlorohexachlorobis[1,1,2,2,2,2-pentachloroethanaminato(2−)]ditungsten, 9CI, 8CI. Di-μ-chlorobis[trichloro(pentachloroethylnitrido)tungsten(VI)]

[32594-38-0]



M 1081.9
Interatomic distance W≡N 171 pm. Synth. from WCl_5 + Cl_3CCN. Orange-yellow cryst. (CH_2Cl_2).

Monomer: Tetrachloro(pentachloroethylimido)tungsten(VI)
C_3Cl_9NW M 540.9
Unknown except as adducts with a wide range of ligands, see eg. Tetrachloro(pentachloroethylimido)(trichloroacetonitrile)tungsten(*VI*), IC-003858.

Drew, M.G.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 231 (*cryst struct*)
Fowles, G.W.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1871 (*synth*)

$C_4CoN_4^{2\ominus}$

Tetrakis(cyano-*C*)cobaltate(2−), 11CI

Tetracyanocobaltate(II)(2−)

$[Co(CN)_4]^{2\ominus}$

M 163.0 (ion)
Rare example of low spin square planar Co(*II*) with a single type of unidentate ligand. Stabilised by large cation. Paramagnetic.

Bis[bis(triphenylphosphine)iminium] salt: [90899-45-9].
Pale blue solid. Sol. MeCN.

Carter, S.J. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 4265 (*synth, ir, magnetism, cryst struct*)

$C_4CoN_4^{\ominus}$

Tetrakis(cyano-*C*)cobaltate(1−), 11CI, 10CI

Tetracyanocobaltate(III)

$[Co(CN)_4]^{\ominus}$

M 163.0 (ion)
Catalyst used in synth. of 1-cyanocycloalkenes.

Ph_4P salt: [63088-02-8].
Synth. by thermal dec. of $[Ph_4P]H_3[Co(CN)_6]$ under N_2 at 210-220°. Turquoise blue cryst. Sol. MeOH, MeCN, DMSO, DMF; insol. H_2O. Ir ν_{CN} 2171, 2137 cm^{-1}. μ_{eff} = 1.85 μ_B (298K).

[86023-82-7]

Papp, S. *et al*, *Z. Naturforsch., B*, 1977, **32**, 167 (*synth, ir, uv-vis*)
Funabiki, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 649 (*use*)

$C_4CoN_4O_3S^{3\ominus}$

Tetrakis(cyano-*C*)sulfitocobaltate(*III*)(3−)

$[Co(CN)_4(SO_3)]^{3\ominus}$

M 243.0 (ion)
Not isol. Probable intermed. in substitution reactions of $[Co(CN)_4(SO_3)(OH_2)]^{3\ominus}$.

Tewari, P.H. *et al*, *Inorg. Chem.*, 1967, **6**, 611.
Wilmarth, W.K. *et al*, *Coord. Chem. Rev.*, 1983, **51**, 209.

$C_4CoN_4O_6S_2^{5\ominus}$

Tetrakis(cyano-*C*)bis(sulfito-*S*)cobaltate(5−), 8CI

Tetracyanodisulfitocobaltate(III)

$[Co(CN)_4(SO_3)_2]^{5\ominus}$

M 323.1 (ion)
trans-Octahedral anion.

Penta-Na salt: [29012-53-1].
Orange-yellow solid. Sol. H_2O.

Chen, H.H. *et al*, *Inorg. Chem.*, 1966, **5**, 1913 (*synth, uv, kinetics, raman*)
Maki, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 2450 (*synth, electrochem*)

$C_4CoN_4S_4^{2\ominus}$

Tetrakis(thiocyanato-*N*)cobaltate(2−)

Tetraisothiocyanatocobaltate(II)

[18904-81-9]

$[Co(NCS)_4]^{2\ominus}$

M 291.2 (ion)
Contains tetrahedrally coord. $Co^{2\oplus}$.

Di-Na salt: [42186-76-5].
Blue cryst. + $8H_2O$.

Di-K salt: [19453-13-5].
Blue cryst. + $4H_2O$. μ_{eff} = 4.38 μ_B (4.47).

Hg(II) *salt:* [27685-51-4].
$C_4CoHgN_4S_4$ M 491.8
Used as calibrant in magnetic susceptibility determinations; also in gravimetric estimation of cobalt. Blue solid.

Bis-Me_4N salt: [14052-14-3].
Blue cryst. Sol. Me_2CO, $PhNO_2$, $MeNO_2$. Mp 197°. μ_{eff} = 4.40 μ_B.

[16039-28-4, 59585-17-0]

Zhdanov, G.S. *et al*, *Zh. Fiz. Khim.*, 1950, **24**, 1339 (*cryst struct*)
Figgis, B.N. *et al*, *J. Chem. Soc.*, 1958, 4190 (*magnetism*)
Holm, R.H. *et al*, *J. Chem. Phys.*, 1960, **32**, 1158 (*magnetism*)
Figgis, B.N., *Trans. Faraday Soc.*, 1960, **56**, 1553 (*magnetism, use*)
Cotton, F.A. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 4157 (*synth, uv-vis, magnetism*)
Vogel, A.I., *Qualitative Inorg. Anal.*, 4th Ed., Longmans, 1978, 461 (*use*)

IC-003865

$C_4CoO_4^{\ominus}$

Tetracarbonylcobaltate(1−), 10CI

Cobalt tetracarbonyl(1−)

[14971-27-8]

$[Co(CO)_4]^{\ominus}$

M 170.9 (ion)
Catalyst for the carbonylation of halohydrocarbons to carboxylic acids, esp. under phase-transfer catalysis condition.
▷ GF9520000.

Li salt: [15616-75-8].
C_4CoLiO_4 M 177.9
White cryst.

Na salt: [14878-28-5].
C_4CoNaO_4 M 193.9
White solid.

K salt: [14878-26-3].
C_4CoKO_4 M 210.0
No phys. props. reported.

In(3+) salt: [15820-67-4].
$C_{12}Co_3InO_{12}$ M 627.7
Red cryst.

Tl(1+) salt: [38991-21-8].
C_4CoO_4Tl M 375.3
Yellow cryst. (H_2O). Mp 120-130° dec. Ir ν_{CO} 2043, 1972, 1937 cm^{-1} (CH_2Cl_2).
▷ Toxic.

Clark, R.J. *et al*, *J. Organomet. Chem.*, 1968, **11**, 637 (*synth*)
Edgell, W.F. *et al*, *Inorg. Chem.*, 1970, **9**, 1932 (*synth*)
Lyford, P. *et al*, *J. Chem. Phys.*, 1970, **52**, 4329 (*synth, ir*)
Edgell, W.F. *et al*, *Ions Ion Pairs Org. React.*, 1972, **1**, 153 (*ir, rev*)
Schlusser, D.P. *et al*, *Inorg. Chem.*, 1974, **13**, 153 (*synth, cryst struct*)
Burlitch, J.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 828 (*synth, ir, ms*)
Habeeb, J.J. *et al*, *Can. J. Chem.*, 1979, **57**, 2196 (*synth, ir*)
Gladysz, J.A. *et al*, *Inorg. Chem.*, 1979, **18**, 553 (*synth, ir*)
Alper, H., *Adv. Organomet. Chem.*, 1981, **19**, 183 (*use, rev*)

IC-003866

$C_4CrNO_5^{\ominus}$

Tetracarbonylnitrosylchromate(1−)

$[Cr(CO)_4NO]^{\ominus}$

M 194.0 (ion)
Trigonal bipyramidal with equatorial NO.

Bis(triphenylphosphine)iminium salt: [116426-70-1].
Red-brown cryst. Ir ν_{CO} 1993, 1895, 1850; ν_{NO} 1608 (1577) cm^{-1} (THF); nmr: $\delta(^{15}N)$ 448.5 ppm (CH_2Cl_2).

Mantell, D.R. *et al*, *J. Organomet. Chem.*, 1988, **347**, 333.

IC-003867

$C_4CrN_4S_4^{2\ominus}$

Tetrakis(thiocyanato-*N*)chromate(*II*)(2−), 10CI

Tetraisothiocyanatochromate(II)(2−)

$[Cr(NCS)_4]^{2\ominus}$

M 284.3 (ion)
Many salts of the kind $A_2[Cr(CNS)_4]$ are known, whose colour/struct. depend on the synthetic conditions.

brown-form
Square planar anion.

Bis-tetrabutylammonium salt: [73494-34-5].
Brown cryst. Insol. H_2O; spar. sol. EtOH. $\mu_{eff} = 4.76\mu_B$ (90-295K).

blue-form
Bis[μ-(thiocyanato-N:S)]hexakis(thiocyanato-N) dichromate(II)(4−)
Dimeric anion with 5-coordinate Cr.

Bis-tetrabutylammonium salt: Blue cryst. V. sol. Me_2CO. Antiferromagnetic.

Larkworthy, L.F. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 262 (*synth, ir, uv, magnetism*)
Larkworthy, L.F. *et al*, *Some Recent Dev. Chem. of Chromium, Molybdenum and Tungsten, Conf. Proc.*, University of Sussex, 1983, L23.

IC-003868

$C_4CrO_4^{4\ominus}$

Tetracarbonylchromate(4−)

$[Cr(CO)_4]^{4\ominus}$

M 164.0 (ion)

Tetra-Na salt: [67202-62-4].
$C_4CrNa_4O_4$ M 255.9
Used to synth. other organometallics. Yellow powder, best used *in situ*. Ir ν_{CO} 1657w, 1462s,br cm^{-1} (silicone mull).
▷ Extremely pyrophoric; may deflagrate or explode.

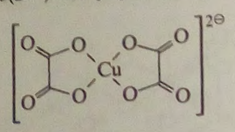
Lin, J.T. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 2296 (*synth, ir, haz, use*)

IC-003869

$C_4CuO_8^{2\ominus}$

Bis(oxalato)cuprate(*II*)(2−)

Bis[ethanedioato(2−)-O,O′]cuprate(2−), 10CI



M 239.5 (ion)

Di-Na salt: [73505-53-0].
Light blue cryst. + $2H_2O$. Exhibits weak antiferromagnetic coupling within chains of stacked $[Cu(C_2O_4)_2]^{2\ominus}$ units.

Di-K salt: [53513-79-4].
Blue cryst. + $2H_2O$.

Propylenediammonium(2+) salt: [78307-66-1].
Royal blue cryst. Anions interact with only 2 neighbours to form linear chain arrangement. Strongly coupled 1D ferromagnetic system.

Bis(benzylammonium) salt: [78307-65-0].
Pale blue platelets. Each anion interacts with 4 neighbours to form infinite layer struct. Weakly coupled 2-D ferromagnet.

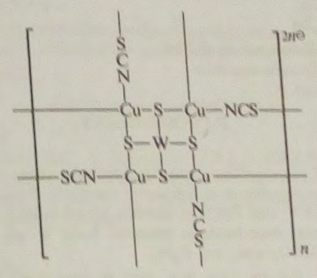
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 991 (*synth, K salt*)
McGregor, K.T. *et al*, *Inorg. Chem.*, 1976, **15**, 2159 (*synth, esr*)
Chananont, P. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 2145.
Gleizes, A. *et al*, *Inorg. Chem.*, 1980, **19**, 2074 (*cryst struct, props, synth*)
Bloomquist, D.R. *et al*, *Inorg. Chem.*, 1981, **20**, 3308 (*cryst struct, props*)
Willet, R.D., *J. Crystal Growth*, 1981, **53**, 437 (*synth*)

$C_4Cu_4N_4S_8W^{2\ominus}$

IC-003870

Tetrakis[(thiocyanato-*N*)cuprate]tetra-μ_3-thioxotungstate(2−), 11CI

Tetrakis(μ_3-sulfido)tetrakis[(μ-isothiocyanato-N,S)copper(I)] tungstate(VI)(2−)



M 798.6 (ion)
Polymeric, solid state struct. dependent on cation. In soln., both salts appear to possess same anion.

Bis-Me_4N salt: [106305-72-0].
Synth. from $(NMe_4)_2WS_4$, CuCl + KSCN in $MeCN/CH_2Cl_2$. Red cryst. Insol. most org. solvs.; sol. DMF. Possesses 3-D polymeric struct., consisting of tetrahedral WS_4 core and four bridging Cu atoms. Ir ν_{CN} 2122, 2087 cm^{-1}.

Bis-Ph_4P salt: [111349-54-3].
Orange microcryst. Sol. DMF, MeCN; insol. Et_2O. In solid state possesses 2-D network of infinite sheets, with PPh_4 cations in between. One Cu atom interacts weakly with S on NCS of adjacent chain to link sheets. Ir ν_{CN} 2109s, 2090s cm^{-1}.

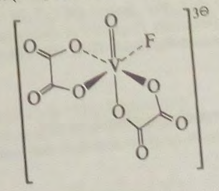
Manoli, J.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 1557 (*cryst struct, ir*)
Potvin, C. *et al*, *Inorg. Chem.*, 1987, **26**, 4370 (*synth, cryst struct, ir, uv-vis*)

IC-003871

$C_4FO_9V^{3\ominus}$

Fluorobis(oxalato)oxovanadate(*IV*)(3−)

Bis[ethanedioato(2−)-O,O′]fluoroxovanadate(3−), 9CI



M 261.9 (ion)
cis-Octahedral struct.

Tri-Na salt: [60125-80-6].
Synth. by dissolving $NaVO_3$ in aq. oxalic acid and adding NaF. Pale blue solid + $6H_2O$.

Tri-NH_4 salt: [60125-81-7].
Synth. similarly to the Na salt.

Reiskamp, H. *et al*, *Z. Naturforsch., B*, 1976, **31**, 537 (*synth, cryst struct*)

IC-003872

$C_4F_3FeO_4P$

Tetracarbonyl(phosphorous trifluoride)iron, 9CI

[16388-47-9]

$Fe(CO)_4PF_3$

M 255.8
Stereochemically nonrigid. Yellow air- and moisture-sensitive liq. Stable in hydrocarbon solvs. attacked rapidly by Me_2CO and EtOH. Immisc. H_2O.

Clark, R.J. *et al*, *Inorg. Chem.*, 1964, **3**, 1395 (*synth*)
Bigorgne, M. *et al*, *Rev. Chim. Minér.*, 1966, **3**, 831 (*ir, raman*)
Haas, H. *et al*, *J. Chem. Phys.*, 1967, **47**, 2996 (*ir*)
Udovich, C.A. *et al*, *Inorg. Chem.*, 1969, **8**, 1066 (*stereochem, nmr*)
Mahnke, H. *et al*, *J. Chem. Phys.*, 1974, **60**, 2997 (*ir, cmr*)
Sheline, R.K. *et al*, *New Synth. Methods*, 1975, **3**, 219 (*synth, ir, nmr*)
Inorg. Synth., 1976, **16**, 63 (*synth*)
Head, R.A. *et al*, *J. Organomet. Chem.*, 1978, **145**, 75 (*pe*)

IC-003873

$C_4F_3O_4PRu$

Tetracarbonyl(trifluorophosphine)ruthenium(0)

Tetracarbonyl(phosphorous trifluoride)ruthenium, 9CI

[36429-98-8]

$Ru(CO)_4(PF_3)$

M 301.0
Identification only tentative - may be an isomeric mixture. A minor product of the reaction between $Ru_3(CO)_{12}$, CO and PF_3 at 150° and high pressure. Light-yellow liq. Ir ν_{CO} 2106, 2087, 2041, 2027, 2008 cm^{-1} (hexane).

Udovich, C.A. *et al*, *J. Organomet. Chem.*, 1972, **36**, 355 (*synth, ir, nmr*)

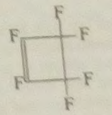
IC-003874

C_4F_6

Hexafluorocyclobutene, 9CI

Fluorocarbon C-1316

[697-11-0]



M 162.0
Fp −60° (−60.4°). Bp 3° (1.1°).
▷ GU1820000.

Hudlický, M., *Chemistry of Organic Fluorine Compounds*, Pergamon, Oxford, 1961, 133, 151, 173, 249 (*reactions*)
Barthes, D. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1974, **279**, 1017.

IC-003875

$C_4F_6HgO_4$

Bis(trifluoroacetato-*O*)mercury

Mercury(II) *trifluoroacetate*

[75513-04-1]

$F_3CCOOHgOOCCF_3$

M 426.6
Transesterification catalyst. Used in mercuration of arenes and oxymercuration of alkenes etc. Cryst. V. sol. DMF, DMSO, Me_2CO, EtOAc, THF, Et_2O, C_6H_6, CH_2Cl_2. Mp 167-169°. Forms $F_3CHgOOCCF_3$ on heating at 300°; photolysis provides $CF_3^{\cdot}$.

[13257-51-7]

Shearer, D.A. *et al*, *Can. J. Chem.*, 1955, **33**, 1002 (*synth, powder struct*)
Brown, H.C. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 5646 (*synth*)
Seyferth, D. *et al*, *J. Organomet. Chem.*, 1974, **72**, 87 (*synth, thermolysis*)

Kagramanov, N.D. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1977, 1835 (*photochem*)
Manhas, B.S. *et al, J. Indian Chem. Soc.*, 1982, **59**, 315 (*ir*)
Baird, W.C. *et al, J. Org. Chem.*, 1985, **50**, 4601 (*synth*)

IC-003876

$C_4F_6Hg_2O_4$

Bis(trifluoroacetato-*O*)dimercury(*I*)
Mercury(I) *trifluoroacetate dimer*
[53154-48-6]

$F_3CCOOHg—HgOOCCF_3$

M 627.2
Discrete molecules connected by Hg...O bonds to form puckered ribbon-like struct. From F_3CCOOH and Hg_2CO_3 in aq. soln. or by electrochemical oxidation of F_3CCOOH at Hg anode at 30-40°. Cryst.

[2923-15-1]

Sevarts, F., *Bull. Soc. Chim. Belg.*, 1939, **48**, 176 (*synth*)
Sikirica, M. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 144 (*cryst struct*)
Ol'dekop, Yu.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1976, **229**, 637 (*synth*)
Ol'dekop, Yu.A. *et al, Zh. Obshch. Khim.*, 1978, **48**, 426 (*synth*)

IC-003877

$C_4F_6MgO_4$

Magnesium trifluoroacetate
Trifluoroacetic acid, magnesium salt, 8CI. 2,2,2-Trifluoroethanoic acid, magnesium salt. Magnesium bis(trifluoroacetate)
[38482-84-7]

$Mg(OOCCF_3)_2$

M 250.3
Synth. by reaction of Mg with trifluoroacetic acid in ethereal solvs. Commercially available as either the bis-(trifluoroacetic acid) adduct or in soln. (1.0 mol l^{-1}) in Et_2O. Reagent used with borane diisopropylamine to reduce selectively polyfunctional ketones. Dec. on heating to form MgF_2.

Faniran, J.A. *et al, Spectrochim. Acta, Part A*, 1976, **32**, 1351 (*ir*)
Karaday, S. *et al, J. Am. Chem. Soc.*, 1981, **103**, 6765 (*uses*)
Reider, P.J. *et al, Tetrahedron Lett.*, 1982, **23**, 2293.
Joosten, P.H. *et al, Appl. Opt.*, 1985, **24**, 2674 (*thermal dec*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2181B, 2181C (*haz*)

IC-003878

$C_4F_6MnO_4$

Manganese(*II*) trifluoroacetate

$Mn(OOCCF_3)_2$

M 280.9
Synth. from $MnCl_2$ and Mn powder in $MeNO_2$ or Et_2O and $AgOOCCF_3$. Pink cryst. Sol. Et_2O, sl. sol. C_6H_6, $MeNO_2$. $\mu_{eff} = 3.50\mu_B$. Forms adducts with Py and PyN-oxide.

Baillie, M.J. *et al, J. Chem. Soc. A*, 1968, 3110 (*synth, ir, uv-vis, magnetism, thermal dec*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 63 (*rev, bibl*)

IC-003879

$C_4F_6O_4Pb$

Lead(*II*) trifluoroacetate
Trifluoroacetic acid, lead(2+) salt, 9CI
[4146-73-0]

$Pb(OOCCF_3)_2$

M 433.2
Hygroscopic cryst.

Faniran, J.A. *et al, Spectrochim. Acta, Part A*, 1976, **32**, 1351 (*ir*)
Indrichan, K.M. *et al, Zh. Neorg. Khim.*, 1984, **29**, 1450; *CA*, **101**, 100765a (*ms*)

IC-003880

$C_4F_6O_4Zn$

Bis(trifluoroacetato-*O*)zinc
Zinc(II) *trifluoroacetate*
[21907-47-1]

$F_3CCOOZnOOCCF_3$

M 291.4
Compd. prepared in aq. soln. is a hydrate; some dec. occurs on attempt to dehydrate thermally. From $AgOOCF_3$ and $ZnCl_2$ in $MeNO_2$. Cross-linking catalyst for epoxy resin-hardener mixtures. Solid. V. sol. H_2O; sol. $MeNO_2$; spar. sol. C_6H_6.

Swarts, F., *Bull. Soc. Chim. Belg.*, 1939, **48**, 176 (*synth*)
Baillie, M.J. *et al, J. Chem. Soc. A*, 1968, 3110 (*synth*)

IC-003881

C_4F_8

Octafluorocyclobutane, 9CI
Perfluorocyclobutane. Fluorocarbon C-318
[115-25-3]

M 200.0
Thermal dimer of $CF_2{=}CF_2$. Refrigerant, polymerisation monomer, heat-transfer medium, propellant (used in foods). Gas. Mp −41.4° (−40.7°). Bp −6.04°.
▷ GU1779500.

U.S. Pat., 2 384 821, (1945); *CA*, 1877, **40** (*synth*)
Lewis, E.E. *et al, J. Am. Chem. Soc.*, 1947, **69**, 1968 (*synth*)
Atkinson, B. *et al, J. Chem. Soc.*, 1953, 2083 (*synth*)
Phillips, W.D., *J. Chem. Phys.*, 1956, **25**, 949 (*nmr*)
Miller, W.T. *et al, J. Am. Chem. Soc.*, 1957, **79**, 3084 (*synth*)
Manuel, T.A., *J. Am. Chem. Soc.*, 1961, **83**, 249 (*synth*)
Chang, C.-H. *et al, J. Mol. Struct.*, 1971, **7**, 89 (*struct*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1007 (*haz*)

IC-003882

$C_4F_{12}HgN_2$

Bis[bis(trifluoromethyl)amino]mercury
*Bis[1,1,1-trifluoro-*N*-(trifluoromethyl)-methanaminato] mercury, 9CI*
[80715-97-5]

$(F_3C)_2NHgN(CF_3)_2$

M 504.6
Solid or liq. at r.t. Mp 17-18°.

Young, J.A. *et al, J. Am. Chem. Soc.*, 1958, **80**, 3604 (*synth*)
Emeleus, H.J. *et al, J. Chem. Soc.*, 1964, 396 (*synth*)

IC-003883

$C_4F_{12}HgN_2S_4$

Bis[bis(trifluoromethylthio)amino]mercury
*1,1,1-Trifluoro-*N*-[(trifluoromethyl)thio]methanesulfenamide mercury(2+) salt (1:1), 9CI*
[61313-71-1]

$Hg[N(SCF_3)_2]_2$

M 632.8
Prepd. from $(CF_3Hg)_2O + (CF_3S)_2NH$.

Fiegler, K.H. *et al, Chem.-Ztg.*, 1976, **100**, 339 (*synth, pmr, F-19 nmr, ms, ir*)

IC-003884

$C_4F_{12}N_2O_8S_4Xe$

Bis[bis(trifluoromethanesulfonyl)amido]xenon
Xenon bis[iminobis[(trifluoromethyl)sulfonate]]
[82113-64-2]

$(F_3CSO_2)_2N—Xe—N(SO_2CF_3)_2$

M 691.5
Synth. from $XeF_2 + Me_3SiN(SO_2CF_3)_2$ in CF_2Cl_2 at 10°. White cryst., stable at 22° under N_2. Dec. at 72°.

Foropoulos, J.J. *et al, J. Am. Chem. Soc.*, 1982, **104**, 4260 (*synth, F-19 nmr, ms, raman*)

IC-003885

$C_4F_{12}N_2S_5$

Tetrakis(trifluoromethylmercapto)diaminosulfane
*N,N′-Thiobis[1,1,1-trifluoro-*N*-[(trifluoromethyl)thio] methanesulfenamide], 9CI*
[53355-89-8]

$(F_3CS)_2NSN(SCF_3)_2$

M 464.3
Synth. from $(F_3CS)_2NH + SCl_2$. Yellow liq.; unstable at r.t. $Bp_{0.2}$ 33°.

Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1974, **406**, 185 (*synth, ir, F-19 nmr, ms*)

IC-003886

$C_4F_{12}N_2S_6$

Tetrakis(trifluoromethylmercapto)diaminodisulfane
*N,N′-Dithiobis[1,1,1-trifluoro-*N*-[(trifluoromethyl)thio] methanesulfenamide], 9CI*
[53355-90-1]

$(F_3CS)_2NSSN(SCF_3)_2$

M 496.4
Formed from $(F_3CS)_2NH + S_2Cl_2$. Yellow liq. $Bp_{0.08}$ 46°. Slowly dec. at r.t.

Haas, A. *et al, Z. Anorg. Allg. Chem.*, 1974, **406**, 185 (*synth, ir, F-19 nmr, ms*)

IC-003887

$C_4F_{12}Te$

Difluorobis(pentafluoroethyl)tellurium
Bis(perfluoroethyl)tellurium difluoride
[51255-76-6]

$(F_3CCF_2)_2TeF_2$

M 403.6
Cryst. solid. Mp 57°. Tetrahedral.

Paige, H.L. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 277 (*synth*)
Lau, C. *et al, Can. J. Chem.*, 1985, **63**, 2273 (*synth, ir, raman, F-19 nmr*)

IC-003888

C_4FeHgO_4

Tetracarbonylmercurioiron, 8CI
[24980-89-0]

$[Hg[Fe(CO)_4]]_n$

M 368.4
Polymeric. Small orange-yellow cryst. Sol. Me_2CO, EtOH, Et_2O, Py, $PhNO_2$.

Hock, H. *et al, Ber.*, 1929, **62**, 431 (*synth, props*)
Beck, W. *et al, J. Organomet. Chem.*, 1967, **10**, 307 (*ir*)
Takano, T. *et al, Bull. Chem. Soc. Jpn.*, 1971, **44**, 431 (*ir, mössbauer*)

IC-003889

$C_4FeI_2O_4$

Tetracarbonyldiiodoiron(*II*), 9CI
Diiodotetracarbonyliron(II). *Tetracarbonyliron diiodide*
[14878-30-9]

$Fe(CO)_4I_2$

M 421.6
Octahedral.

cis-form [14911-55-8]
Red-black cryst. *trans*-form also known.

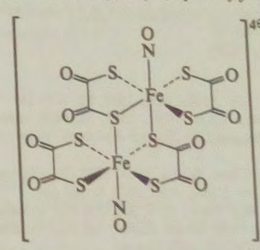
trans-form [15616-56-5]

Hieber, W. *et al, Ber.*, 1928, **61**, 1717.
Baraclough, C.C. *et al, J. Chem. Soc.*, 1961, 2582 (*ir*)
Noack, K., *Helv. Chim. Acta*, 1962, **45**, 1847 (*ir*)
Lewis, J. *et al, Acc. Chem. Res.*, 1968, **1**, 245 (*ms*)
Panowski, M. *et al, J. Organomet. Chem.*, 1969, **19**, 393 (*synth, ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1956 (*synth*)
Vancea, L. *et al, J. Organomet. Chem.*, 1977, **134**, 219 (*cmr*)

IC-003890

$C_4FeNO_5S_4^{2\ominus}$

Bis(dithiooxalato)nitrosylferrate(2−)
Bis[ethanebis(thioato)(2−)-S,S′]nitrosylferrate(2−)



dimer

M 326.1 (ion)
Dimeric. Synth. from $Fe(S_2C_2O_2)_3^{3\ominus}$ salts heated to 70° in aq. $NaNO_2$ or $MeNO_2$. Superexchange mechanism present between Fe centres.

Dimer, tetra-K salt: [125472-08-4].
$C_8Fe_2K_4N_2O_{10}S_8$ M 808.7
Synth. from aq. $K_2C_2O_2S_2 + FeCl_3.6H_2O$ followed by addn. of KNO_2. Black cryst. + $2H_2O$ (H_2O). Sol. H_2O.
Dimer, tetrakis(benzyltriphenylphosphonium) salt: Green cryst. Mp 158-161°. $\mu_{eff} = 2.22\mu_B$.

Coucouvanis, D. *et al, J. Am. Chem. Soc.*, 1970, **92**, 5004 (*synth, esr, magnetism*)
Birchall, T. *et al, Inorg. Chem.*, 1976, **15**, 376 (*mössbauer*)
Qian, L. *et al, Inorg. Chem.*, 1990, **29**, 761 (*synth, struct, esr, magnetism*)

IC-003891

$C_4FeN_4O_4^{2\ominus}$

Tetrakis(cyanato-*N*)ferrate(2−)
Tetrakis(isocyanato)ferrate(II)(2−)

$[Fe(NCO)_4]^{2\ominus}$ (T_d)

M 223.9 (ion)
Bis-Et_4N salt: Pale brown solid (impure due to easy oxidn.); hygroscopic.

Forster, D. *et al, J. Chem. Soc.*, 1965, 262, 454 (*ir, synth*)

$C_4FeN_4O_4^{\ominus}$ – $C_4HFeO_4^{\ominus}$

$C_4FeN_4O_4^{\ominus}$ IC-003892

Tetrakis(cyanato-*N*)ferrate(1−)

Tetrakis(isocyanato)ferrate(III)(*1−*)

$[Fe(NCO)_4]^{\ominus}$ (T_d)

M 223.9 (ion)

Et_4N salt: [21279-20-9].
Sol. MeCN.

Ph_4As salt: Synth. from $[Ph_4As][FeCl_4]$ + AgNCO in Me_2CO. Orange cryst. (Me_2CO). Mp 159°.

Forster, D. *et al, J. Chem. Soc.*, 1965, 262 (*ir, synth*)
Day, P., *Inorg. Chem.*, 1966, **5**, 1619 (*uv*)
Edwards, P.R. *et al, J. Chem. Phys.*, 1968, **49**, 211 (*mössbauer*)

$C_4FeO_4^{2\ominus}$ IC-003893

Tetracarbonylferrate(2−)

Collman's reagent

[51222-96-9]

$[Fe(CO)_4]^{2\ominus}$ (T_d)

M 167.8 (ion)
Used in org. synth. as a transition metal analogue of Grignard reagents. Sol. THF (0.007 mol dm^{-3}). pK_a 14. Ir ν_{CO} 1730 cm^{-1}.

Di-Na salt: [14878-31-0].
Usually generated and used *in situ*. V. air-sensitive orange cryst. (MeOH/THF). Forms cryst. dioxan adduct.

Di-K salt: [16182-63-1].
Cryst. (MeOH/THF).

[22321-35-3]

Edgel, W.F. *et al, J. Am. Chem. Soc.*, 1960, **82**, 1254 (*ir*)
Stammreich, H. *et al, J. Chem. Phys.*, 1960, **32**, 1482 (*raman*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 216 (*uses*)
Greatrex, R. *et al, J. Chem. Soc. A*, 1969, 2339 (*ir, mössbauer*)
Collman, J.P. *et al, Acc. Chem. Res.*, 1975, **8**, 342 (*rev*)
Baerends, E.J. *et al, Mol. Phys.*, 1975, **30**, 1735 (*uv, ir, raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1829 (*synth*)
Teller, R.G. *et al, J. Am. Chem. Soc.*, 1977, **99**, 1104 (*struct*)
Collman, J.P. *et al, J. Am. Chem. Soc.*, 1977, **99**, 1104, 2515 (*synth, cryst struct*)
Collman, J.P. *et al, J. Am. Chem. Soc.*, 1977, **99**, 2515 (*synth, solv*)
Ernst, R.D. *et al, Inorg. Chem.*, 1978, **17**, 1477 (*synth, derivs*)
Pensak, D.A. *et al, Inorg. Chem.*, 1979, **18**, 3407 (*struct*)
Cymbaluk, T.H. *et al, Inorg. Chem.*, 1980, **19**, 2381 (*synth*)
Org. Synth., 1980, **59**, 102 (*synth, use*)
Bowen, P. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 679 (*synth*)
Inorg. Synth., 1986, **24**, 157 (*synth*)

C_4FeO_4Zn IC-003894

Tetracarbonyl(zinc)iron, 9CI

Tetracarbonylzinciotron, 8CI

[32458-92-7]

$Zn[Fe(CO)_4]$

M 233.2
Prepd. in aq. soln. and not isol.

Gsiembeck, F. *et al, J. Am. Chem. Soc.*, 1971, **93**, 1909 (*synth*)

$C_4GeN_4O_4$ IC-003895

Germanium(*IV*) isocyanate

Tetrakis(cyanato-N)germanium. Tetraisocyanatogermane

[4756-66-5]

$Ge(NCO)_4$

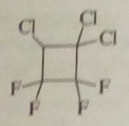
M 240.6
Prepd. from $GeCl_4$ + AgCNO in C_6H_6. Colourless liq. Rapidly hydrol. d^{24} 1.7694. Mp −8°. Bp 204°. n_D^{25} 1.4793. Corresp. cyanate compd. unknown.

Laubengayer, A.W. *et al, J. Am. Chem. Soc.*, 1943, **65**, 1783 (*synth*)
Forbes, G.S. *et al, J. Am. Chem. Soc.*, 1943, **65**, 2271 (*synth*)
Miller, F.A. *et al, Spectrochim. Acta*, 1961, **17**, 977 (*ir, raman*)

$C_4HCl_3F_4$ IC-003896

1,1,4-Trichloro-2,2,3,3-tetrafluorocyclobutane

Fluorocarbon C-324



M 231.4

(±)-form
Synth. by the cycloaddition reaction of $CF_2{=}CF_2$ and $CCl_2{=}CHCl$. d_4^{25} 1.572. Bp 109-110.5°. n_D^{25} 1.3995.

Coffman, D.D. *et al, J. Am. Chem. Soc.*, 1949, **71**, 490 (*synth*)

$C_4HF_9O_6S_3$ IC-003897

Tris(trifluoromethylsulfonyl)methane

[60805-12-1]

$HC(SO_2CF_3)_3$

M 412.2
Synth. from CF_3SO_2F and MeMgBr via $CH_2(SO_2CF_3)_2$. V. strong acid. Colourless, v. hygroscopic solid. Mp 69.2°.

K salt: [114395-69-6].
Synth. from $HC(SO_2CF_3)_3$ and K_2CO_3. Colourless needle-shaped cryst.

Rb salt: [114395-70-9].
Synth. from $HC(SO_2CF_3)_3$ and Rb_2CO_3. Colourless cryst.

Cs salt: [114395-68-5].
Synth. from $HC(SO_2CF_3)_3$ and Cs_2CO_3. Colourless cryst. (hot H_2O). Spar. sol. H_2O. Subl. 30° *in vacuo*.

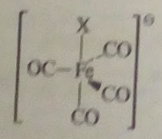
Ag salt: [114395-71-0].
Synth. from $HC(SO_2CF_3)_3$ and Ag_2CO_3. Colourless cryst. turns brown in air.

Turowsky, L. *et al, Inorg. Chem.*, 1988, **27**, 2135 (*synth, salts, reactions, ir*)

$C_4HFeO_4^{\ominus}$ IC-003898

Tetracarbonylhydroferrate(1−), 9CI, 8CI

[18716-80-8]



X = H

M 168.8 (ion)
Used in org. reductions; $Na^{\oplus}$ and $K^{\oplus}$ derivs. usually prepd. and used *in situ* without isol.

Na salt: [53558-55-7].
$C_4HFeNaO_4$ M 191.8
Obt. quantitatively in THF from $Na_2Fe(CO)_4$ with 1 equiv. AcOH. White solid. Forms 1:1 solvate with MeOH and EtOH.

C_4HIrO_4 – $C_4H_2Cl_4Ir_2O_4$

Me_4N salt: [63814-56-2].
Light-pink cryst. Mod. air-sensitive.

Bis(triphenylphosphine)iminium salt: [56791-54-9].
$C_{40}H_{31}FeNO_4P_2$ M 707.4
V. pale-yellow plates (EtOH/EtOAc).

Methyltriphenylphosphonium salt: Pale-yellow cryst. (butanol). Mp 90°.

Edgell, W.F. *et al, J. Am. Chem. Soc.*, 1960, **82**, 1254 (*ir*)
Stammreich, H. *et al, J. Chem. Phys.*, 1960, **32**, 1482 (*raman*)
Smith, M.B. *et al, J. Am. Chem. Soc.*, 1973, **95**, 2388 (*cryst struct*)
Mitsudo, T. *et al, Chem. Lett.*, 1974, 1358 (*pmr*)
Siegl, W.O. *et al, J. Organomet. Chem.*, 1975, **92**, 321 (*synth*)
Pettit, R. *et al, Tetrahedron Lett.*, 1977, 781 (*synth, bibl*)
Collman, J.P. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1119 (*synth, bibl*)
Pensak, D.A. *et al, Inorg. Chem.*, 1979, **18**, 3407 (*struct*)
Sósinsky, B.A. *et al, Inorg. Chem.*, 1982, **21**, 4229 (*mössbauer*)
Blyholder, G. *et al, Organometallics*, 1985, **4**, 2170 (*theory, isom*)

C_4HIrO_4 IC-003899

Tetracarbonylhydroiridium, 10CI

Hydridotetracarbonyliridium. Tetracarbonyliridium hydride

[25282-12-6]

$HIr(CO)_4$

M 305.2
Formed under high pressure from $Ir_4(CO)_{12}$, CO and H_2. Dec. to $Ir_4(CO)_{12}$ on removal of pressure. Ir ν_{CO} 2054m, 2031s, 1999w cm^{-1} (pet. ether).

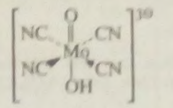
Whyman, R., *J. Chem. Soc., Dalton Trans.*, 1972, 2294 (*synth, ir*)
Vidal, J.L. *et al, Inorg. Chem.*, 1981, **20**, 249 (*synth, ir*)

$C_4HMoN_4O_2^{3\ominus}$ IC-003900

Tetrakis(cyano-*C*)hydroxyoxomolybdate(3−), 9CI

Oxohydroxotetracyanomolybdate(IV)(*3−*)

[36594-14-6]



M 233.0 (ion)
Octahedral anion.

trans-form [52920-70-4]
Blue molybdate ion is the primary aq. sp. present from pH10 - pH13: $[MoO(OH)(CN)_4]^{3\ominus} + H_2O \rightleftharpoons [MoO(H_2O)(CN)_4]^{2\ominus} + OH^{\ominus}$.

Tri-K salt: [55493-42-0].
Blue solid.

Tris(ethylenediamine)chromium(III) *salt:* [55493-44-2].
$C_{10}H_{35}CrMoN_{10}O_3$ M 465.3
Cryst.

[52523-86-1]

Stadnicka, K., *Pol. J. Chem. (Rocz. Chem.)*, 1973, **47**, 2021 (*cryst struct, Na tetrahydrate*)
Mitra, R.P. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 3739 (*spectra*)
Robinson, P.R. *et al, Inorg. Chem.*, 1975, **14**, 203, 2035 (*cryst struct, synth, bibl, ir*)
Young, C.G. *et al, Inorg. Chem.*, 1985, **24**, 4416 (*Mo-95 nmr*)

$C_4HO_4Os^{\ominus}$ IC-003901

Tetracarbonylhydroosmate(1−)

$[HOs(CO)_4]^{\ominus}$

M 303.2 (ion)

Na salt: [22533-60-4].

C_4HNaO_4Os M 326.2
Strong nucleophile. Yellow or cream air-stable solid. Sol. H_2O.

K salt: [80462-68-6].
C_4HKO_4Os M 342.3
Pale yellow powder.

Bis(triphenylphosphine)iminium salt: [79408-53-0].
Colourless cryst. (THF/hexane).

L'Eplattinier, F. *et al, Inorg. Chem.*, 1969, **8**, 965; *Helv. Chim. Acta*, 1973, **53**, 1091 (*synth, ir, pmr, derivs*)
George, R.D. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 972 (*synth, ir*)
Walker, H.W. *et al, Inorg. Chem.*, 1982, **21**, 2509 (*synth, ir, pmr*)
Jordan, R.F. *et al, J. Am. Chem. Soc.*, 1982, **104**, 1255 (*synth, ir, deriv*)

$C_4H_2Br_4O_5Zr$ IC-003902

Bis(dibromoacetato-*O,O'*)oxozirconium(*IV*), 11CI

[97894-99-0]

$(Br_2CHCOO)_2ZrO$

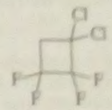
M 540.8
Synth. from $ZrOCl_2$ + $Br_2CHCOOH$. Air-stable white solid + 1 $Br_2CHCOOH$. Sol. $MeNO_2$. Mp >270°.

Puri, J.K. *et al, Inorg. Chim. Acta*, 1985, **101**, 135 (*synth, ir, pmr, cmr*)

$C_4H_2Cl_2F_4$ IC-003903

1,1-Dichloro-2,2,3,3-tetrafluorocyclobutane

Fluorocarbon C-334



M 196.9
Synth. by the cycloaddition reaction of $CF_2{=}CF_2$ and $CH_2{=}CCl_2$. d_4^{25} 1.530. Bp 84-84.7°. n_D^{25} 1.3702.

Coffman, D.D. *et al, J. Am. Chem. Soc.*, 1949, **71**, 490 (*synth*)

$C_4H_2Cl_4Ir_2O_4$ IC-003904

Tetracarbonyldi-μ-chlorodichlorodihydrodiiridium

Di-μ-chlorodichlorodihydrotetracarbonyldiiridium. Tetracarbonyltetrachlorodihydrodiiridium

$[IrHCl_2(CO)_2]_2$

M 640.3
Bronze needles (EtOH), probably dihydrate. Mp >192° dec. Ir ν_{NH} 2105, ν_{CO} 2077, 2044 cm^{-1} (KCl).

Monomer: Dicarbonyldichlorohydridoiridium
$C_2HCl_2IrO_2$ M 320.1
Unknown.

Shaw, B.L. *et al, J. Chem. Soc. A*, 1967, 1683 (*synth, ir*)

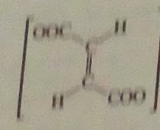
IC-003905

$C_4H_2FeO_4$

Iron(*II*) fumarate

Ferrous fumarate, USAN. Iron(II) (*E*)-*1,3*-*butenedioate.*
Feostat. Ferrocap. Toleron. Numerous proprietary names

[141-01-5]



M 169.9
Synth. from $FeSO_4$ + Na fumarate in H_2O. Haematinic. Air-stable red-brown solid. Insol. EtOH; sl. sol. H_2O. Mp >280°.
B-LT1930000.

[7705-12-6]

Weaver, *et al*, *Am. J. Med. Sci.*, 1961, **241**, 396 (*tox*)
Prabhakaran, P. *et al*, *Indian J. Chem.*, 1969, **7**, 266 (*synth*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 3034.

IC-003906

$C_4H_2FeO_4$

Tetracarbonyldihydroiron, 9CI

Tetracarbonyliron dihydride

[12002-28-7]

$H_2Fe(CO)_4$

M 169.9
Octahedral, stereochemically nonrigid. pK_{a1} 11.4 (25°, MeCN).

cis-form [22763-20-8]
White cryst. melting to a colourless, mobile liq. Mp −70°. pK_{a1} 4.44; pK_{a2} 14.00 (0°). Dec. at −10°. Acidic; forms insol. stable salts with large cations.

Hieber, W. *et al*, *Z. Elektrochem.*, 1953, **57**, 235.
Piper, T.S. *et al*, *J. Inorg. Nucl. Chem.*, 1956, **3**, 104 (*pmr*)
Fatmery, K. *et al*, *J. Chem. Soc. A*, 1970, 634 (*synth, ir*)
Stobart, S.R., *J. Chem. Soc., Dalton Trans.*, 1972, 2442 (*synth, ir, raman*)
McNeill, E.A. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 6243 (*struct*)
Vancea, L. *et al*, *J. Organomet. Chem.*, 1977, **134**, 219 (*synth, cmr*)
Gmelin Handbook Inorg. Chem., 8th Edn., 1978, **B2**, 7 (*bibl*)
Moore, E.J. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2257 (*ir, props*)

$C_4H_2MoN_4O_2^{2\ominus}$

IC-003907

Aquatetrakis(cyano-*C*)oxomolybdate(*IV*)(2−), 9CI

Oxoaquotetracyanomolybdate(2−)

[57298-65-4]

$[MoO(OH_2)(CN)_4]^{2\ominus}$

M 234.0 (ion)
Octahedral anion. Model for nitrogenase systems.

Trans-form

Di-K salt: [59808-17-2].
Sol. H_2O. Attempted isol. gave polymeric products.

Cd salt: [77370-93-5].
$C_4H_2CdMoN_4O_2$ M 346.4
Violet-blue cryst. + $6H_2O$. Previously formulated as $Cd[Mo(OH)_2(CN)_4].6H_2O$. On drying *in vacuo* loses H_2O and becomes grey-brown.

Bis(ethylenediamine)platinum(II) *salt:* [55493-47-5].
$C_8H_{18}MoN_8O_2Pt$ M 549.3
Blue cryst. + $2H_2O$.

Ni(II) *salt:* [98119-01-8].
Dark green solid + $2H_2O$.

Zn(II) *salt:* [98119-00-7].
Brown solid + $2H_2O$.

Co(II) *salt:* [97698-43-6].
$C_4H_2CoMoN_4O_2$ M 292.9
Synth. from $CoCl_2$ and photochemically-generated K salt of anion. Green solid + $2H_2O$.

Bis-Ph_4P salt: [86568-28-7].
Monoclinic green cryst. + $4H_2O$. Ir $\nu_{Mo=O}$ 920 cm^{-1}, Mo=O 172 pm.

Bis-Ph_4As salt: [86568-29-8].
Monoclinic blue cryst. + $4H_2O$. Ir $\nu_{Mo=O}$ 980 cm^{-1}, Mo=O 160 pm.

[21729-48-6, 21729-49-7]

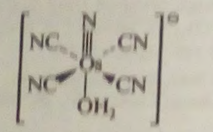
Robinson, P.R. *et al*, *Inorg. Chem.*, 1975, **14**, 2035.
Schrauzer, G.N. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 7069 (*nitrogenase model*)
Dudek, M. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **42**, 1701 (*synth, diagn, ir, raman, uv-vis*)
Wieghardt, K. *et al*, *Z. Anorg. Allg. Chem.*, 1983, **499**, 44 (*synth, cryst struct, uv-vis, ir*)
Ali, S.I. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1985, **15**, 425 (*Co, Ni, Zn salts*)

$C_4H_2N_5OOs^{\ominus}$

IC-003908

Aquatetrakis(cyano-*C*)nitridoosmate(*VI*)(1−)

Aquatetracyanonitridoosmate(VI)(*1−*)



M 326.2 (ion)
trans-Octahedral (C_{4v} symmetry).

K salt: [27216-80-4].
Synth. from K_2OsO_4 and HCN in H_2O. Black cryst. + $2H_2O$. Ir ν_{O-H} 3367s, $\nu_{C\equiv N}$ 2155w, 2070vs, $\nu_{Os\equiv N}$ 1085s, ν_{Os-ON_3} 326m cm^{-1}.

[19633-46-6]

Griffith, W.P., *J. Chem. Soc.*, 1965, 3694 (*synth, ir*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1970, 1117 (*ir*)

$C_4H_2N_5O_3Rh^{2\ominus}$

IC-003909

Aquatetrakis(cyano-*C*)nitritorhodate(*III*)(2−)

Aquatetracyanonitrorhodate(III)(*2−*)

$[Rh(CN)_4(OH_2)(NO_2)]^{2\ominus}$

M 270.9 (ion)
Probably has *trans*-config.

Di-K salt: Synth. from NO_2 and $K_2[RhH(CN)_4(OH_2)]$.

Lawson, D.N. *et al*, *J. Chem. Soc. A*, 1966, 52 (*synth, ir*)

$C_4H_2O_4Os$

IC-003910

Tetracarbonyldihydroosmium, 9CI, 8CI

Osmium carbonyl hydride

[22372-70-9]

As Dibromotetracarbonylosmium, IC-003818 with

X = Y = H

M 304.2
Synth. from $Na_2[Os(CO)_4]$ and an excess of H_3PO_4. Precursor for CO hydrogenation catalyst. Colourless air-stable liq. Mp −40° to −38°. pK_a 12.8 (MeOH, 25°).

[18972-42-4]

Muetterties, E.L., *Transition Metal Hydrides*, Marcel Dekker, New York, 1971.
Kaesz, H.D. *et al*, *Chem. Rev.*, 1972, **72**, 231 (*rev*)
George, R.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 972 (*synth, ir, pmr*)
Collman, J.P. *et al*, *Inorg. Chem.*, 1974, **13**, 1 (*synth, ir*)
Moss, J.R. *et al*, *Inorg. Chem.*, 1977, **16**, 75 (*synth*)
Vancea, P. *et al*, *J. Organomet. Chem.*, 1977, **134**, 219 (*cmr*)
Walker, H.W. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 7428.
Kaesz, H.D. *et al*, *Prog. Inorg. Chem.*, 1979, **25**, 145 (*rev*)
Carter, W.J. *et al*, *Inorg. Chem.*, 1982, **21**, 3955 (*synth, ir, pmr*)
Clark, W.J. *et al*, *Inorg. Chem.*, 1982, **21**, 3955 (*synth, ir, pmr*)
Nicholls, J.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1395 (*synth, ir*)
Carter, W.J. *et al*, *Organometallics*, 1985, **4**, 1376 (*kinetics*)
Lamb, H.H. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 81 (*uv, catalysis*)
Nixon, J.F. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 765 (*pe*)

$C_4H_2O_4Ru$

IC-003911

Tetracarbonyldihydroruthenium, 9CI, 8CI

[21029-23-2]

As Dibromotetracarbonylruthenium, IC-003820 with

X = H

M 215.1
pK_a 18.7.

cis-form [42781-58-8]
V. volatile colourless liq. Mp *ca.* −63°.

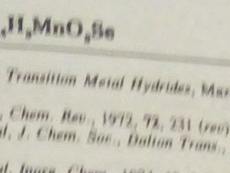
Cotton, J.D. *et al*, *J. Chem. Soc. A*, 1968, 2162 (*synth, ir*)
Whyman, R., *J. Organomet. Chem.*, 1973, **56**, 339 (*ir*)
Bradley, G.F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 325 (*struct, raman*)
Moore, E.J. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2257 (*ir, props, pmr*)

$C_4H_2O_{10}V^{2\ominus}$

IC-003912

Aquabis(oxalato)oxovanadate(*IV*)(2−)

Aquabis[ethanedioato(2−)-O,O′]oxovanadate(IV)(*2−*), *11CI*



M 260.9 (ion)
Distorted octahedral.

Di-NH_4 salt: [104120-69-6].
Synth. from NH_4VO_3 in boiling aq. oxalic acid/ammonium oxalate. Blue-grey cryst. + $1H_2O$ (EtOH aq.). The anhydrous phase appears to be unknown.

[38883-77-1]

Koppell, J. *et al*, *Z. Anorg. Allg. Chem.*, 1903, **36**, 281 (*synth*)
Palmer, W.G., *Experimental Inorganic Chemistry*, Cambridge University Press, 1954, 319 (*synth*)
Oughtred, R.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1972, 945 (*cryst struct*)
Oughtred, R.E. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 82 (*cryst struct*)
Hallmeier, K.H. *et al*, *Spectrochim. Acta, Part A*, 1986, **42**, 841 (*xanes*)

$C_4H_3Ca_4KNa_4O_{32}Si_8$

IC-003913

Carletonite, 9CI

[11092-27-6]

$Na_4KCa_4[Si_8O_{18}][CO_3]_4(OH,F).H_2O$

M 1079.1
Mineral. A branched double layer silicate. Occurs in thermally metamorphosed inclusions in the nepheline syenite at Mont St. Hilaire, Quebec. Pink to pale blue flakes.

Chao, G.Y., *Am. Mineral.*, 1971, **56**, 1855; 1972, **57**, 765 (*mineral, cryst struct*)

$C_4H_3FeO_4P$

IC-003914

Tetracarbonyl(phosphine)iron, 8CI

[18116-52-4]

$Fe(CO)_4PH_3$

M 201.8
Light-yellow needles (pentane). Mp 36°. V. sensitive to oxygen and light.

Fischer, E.O. *et al*, *Chem. Ber.*, 1960, **103**, 2547 (*synth, ir, pmr*)
Bigorgne, M. *et al*, *J. Organomet. Chem.*, 1970, **23**, 201 (*raman, ir*)

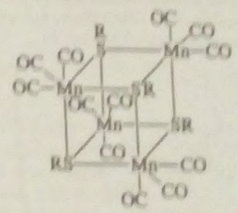
$C_4H_3MnO_3S$

IC-003915

Tricarbonyl(methanethiolato)manganese

Tricarbonyl(methylthio)manganese

[30999-92-9]



Tetramer
R = Me

M 186.0
Tetrameric in soln. Whether tetrameric or trimeric as solid is solv. and prep. dependent. Synth. from $Mn_2(CO)_{10}$ and methyl thiocyanate in refluxing toluene.

Trimer:
$C_{12}H_9Mn_3O_9S_3$ M 558.2

Tetramer: [24819-01-0]. *Dodecacarbonyltetrakis(μ_3-methanethiolato)tetramanganese, 9CI*
$C_{16}H_{12}Mn_4O_{12}S_4$ M 744.2
Yellow-orange cryst. Ir ν_{CO} 2020vs, 2011w, 1947vs, 1906vw (cyclohexane).

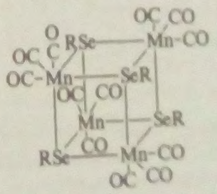
Abel, E.W. *et al*, *J. Chem. Soc. A*, 1966, 1141 (*synth*)
Johnson, B.F.G. *et al*, *Inorg. Chem.*, 1968, **7**, 831 (*ms, synth, pmr*)
Jenkins, C.R., *J. Organomet. Chem.*, 1968, **15**, 441.

$C_4H_3MnO_3Se$

IC-003916

Tricarbonyl(methaneselenolato)manganese

Tricarbonyl(methylseleno)manganese



Tetramer
R = Me

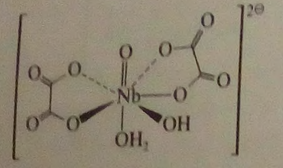
M 232.9
Tetrameric. Synth. by heating $[Mn(SeMe)(CO)_4]_2$ in cyclohexane.
Tetramer: [12302-42-0]. *Dodecacarbonyltetrakis(μ_3-methaneselenolato)tetramanganese*
$C_{16}H_{12}Mn_4O_{12}Se_4$ M 931.8
Orange-brown cryst. (C_6H_6). Mp 190° dec. Ir ν_{CO} 2015vs, 2007vw, 1944s cm^{-1} (cyclohexane).
Abel, E.W. *et al, J. Chem. Soc. A*, 1967, 2014 (*synth, ir, pmr, struct*)

$C_4H_3N_4O_3Rh^{2\ominus}$ IC-003917
Aquatetrakis(cyano-*C*)(hydroperoxy)rhodate(*III*)(2−)
Hydroperoxotetracyanoaquarhodate(III)

$[(H_2O)Rh(CN)_4(OOH)]^{2\ominus}$

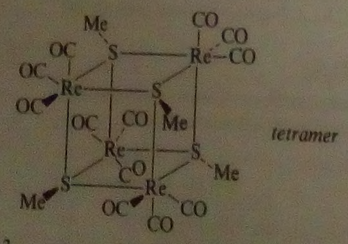
M 257.9 (ion)
Acid hydrol. yields the diaqua complex $[Rh(CN)_4(H_2O)_2]^{\ominus}$ and H_2O_2.
Lawson, D.N. *et al, J. Chem. Soc. A*, 1966, 52 (*synth*)
Roberts, H.L. *et al, J. Chem. Soc. A*, 1968, 1450.

$C_4H_3NbO_{11}^{2\ominus}$ IC-003918
Aquahydroxybis(oxalato)oxoniobate(*V*)(2−)
Aquabis[ethanedioato(2−)-O,O′]hydroxyoxoniobate(V)(2−). *Aquooxohydroxobis(oxalato)niobate*(V)



M 319.9 (ion)
Pentagonal bipyramidal. Other salts have been briefly described by Brnicević.
Di-H compd., pentahydrate: [30553-79-8].
Oxohydroxobis(oxalato)niobic acid
$C_4H_{15}NbO_{16}$ M 412.0
Synth. by crystallisation from aq. solns. containing Nb and oxalate. Colourless solid (H_2O).
Cs, H salt, trihydrate: [30374-59-5].
Synth. from the H compd. + CsOH. Colourless solid.
Brnicević, N. *et al, J. Less-Common Met.*, 1971, **23**, 107 (*synth*)
Galešić, N. *et al, J. Less-Common Met.*, 1971, **25**, 234 (*cryst struct*)

$C_4H_3O_3ReS$ IC-003919
Tricarbonyl(methanethiolato)rhenium(*I*)



tetramer

M 317.3
Tetrameric, originally thought to be trimeric.
Tetramer: [23591-73-3]. *Dodecacarbonyltetrakis(μ_3-methanethiolato)tetrarhenium, 8CI*
$C_{16}H_{12}O_{12}Re_4S_4$ M 1269.3
Synth. from $Me_2Sn(SMe)_2$ and $Re(CO)_5Cl$. Pale yellow cryst. ($CHCl_3$/hexane). Ir ν_{CO} 2028s, 2019w, 1944vs, 1902w cm^{-1} (cyclohexane).
Abel, E.W. *et al, J. Chem. Soc. A*, 1966, 1141 (*synth, ir, pmr*)
Harrison, W. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1009 (*cryst struct*)

$C_4H_3O_4Ru$ IC-003920
(Acetato-*O*)dicarbonylruthenium, 10CI
Dicarbonyl(ethanoato)ruthenium(I)
[26317-70-4]

$[Ru(CO)_2OAc]_\infty$

M 216.1
Formulated as an infinite chain polymer with bridging acetate ligands. Prepd. either by treating $Ru_3(CO)_{12}$ with HOAc (neat or in C_6H_6) at reflux, or by treating $RuCl_3.xH_2O$/NaOAc/HOAc/PrOH with CO (1 atm.). Catalyses the isom. of alkenes or the carbonylation of secondary amines. Yellow amorphous solid; involatile. Insol. non-coordinating solvs. Ir ν_{CO} 2049, 1994, 1967, 1952, 1916, 1908 cm^{-1} (nujol).
Crooks, G.R. *et al, J. Chem. Soc. A*, 1969, 2761 (*synth, ir*)
James, B.R. *et al, Chem. Ind. (London)*, 1971, 1036 (*synth*)
Byerley, J.J. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 1482 (*catalysis*)
Rempel, G.L. *et al, Adv. Chem. Ser.*, 1974, **132**, 166 (*catalysis*)
Braca, G. *et al, Proc. Int. Congr. Catal., 6th*, 1976, **1**, 528 (*ir, catalysis*)

$C_4H_4CdO_6$ IC-003921
Cadmium tartrate
Cadmium 2,3-dihydroxybutanedioate
[10471-46-2]

$Cd(OOCCHOHCHOHCOO)$

M 260.4
Polym. catalyst for episulfides; cross-linking catalyst. Solid. Sl. sol. H_2O. Dec. at 280-370° to CdO.
Pentahydrate: [40302-14-5].
Cryst. Dehydrates at 55-120°.
Pickering, S.U., *J. Chem. Soc.*, 1916, **109**, 235.
Spacu, G. *et al, Z. Anorg. Allg. Chem.*, 1936, **227**, 385.
Gmelin Handbook Inorg. Chem., Syst. No. 33, 1959, 655 (*rev, bibl*)
Kubecova, K. *et al, Collect. Czech. Chem. Commun.*, 1969, **34**, 1141 (*synth, powder struct, ir, hydrate*)
Frei, V. *et al, Collect. Czech. Chem. Commun.*, 1969, **34**, 1304 (*thermal anal, hydrate*)
Andreev, B.Ya. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 291 (*therm anal, synth, hydrate*)
Hopewood, J.S. *et al, J. Appl. Crystallogr.*, 1972, **5**, 437 (*cryst struct, hydrate*)
Yamashita, H., *Bull. Chem. Soc. Jpn.*, 1988, **61**, 1213 (*synth*)

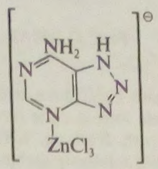
$C_4H_4Cl_2O_5Ti$ IC-003922
Bis(chloroacetato-*O*)oxotitanium(*IV*), 11CI
[104007-38-7]

$TiO(OOCCH_2Cl)_2$

M 250.8
Synth. by reaction of $TiCl_4$ and chloroacetic acid in refluxing CCl_4. White, v. moisture-sensitive solid.
Py complex: [104854-08-2]. *Bis(chloroacetato-O)oxo(pyridine)titanium*(IV), *11CI*
$C_9H_9Cl_2NO_5Ti$ M 329.9

White solid.
Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1986, **25**, 271 (*synth, ir, deriv*)

$C_4H_4Cl_3N_6Zn^{\ominus}$ IC-003923
(8-Azaadenine)trichlorozincate(1−)
Trichloro(1H-1,2,3-triazolo[4,5-d]pyrimidin-7-amine)zincate(1−)



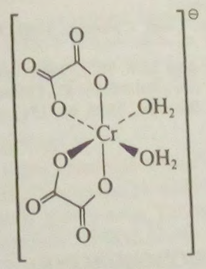
M 307.8 (ion)
H compd.: [63313-01-9]. *(8-Azaadeninium)trichlorozinc*
$C_4H_5Cl_3N_6Zn$ M 308.8
Cryst. (aq. acid). Struct. comprises monomeric units connected by H-bonds.
Purnell, L.G. *et al, J. Am. Chem. Soc.*, 1977, **99**, 3651 (*synth, cryst struct*)

$C_4H_4Cl_{10}N_2Nb_2S_2$ IC-003924
Decachloro[μ-(1,2-ethanediyldithiocyanato-*N*:*N*′)]diniobium(*V*), 10CI
[65139-57-3]

$Cl_5Nb{-}NCSCH_2CH_2SCN{-}NbCl_5$

M 684.5
Synth. from $NbCl_5$ and the ligand in CCl_4. Yellow solid. Mp 181°.
Droll, H.A. *et al, Inorg. Chim. Acta*, 1977, **24**, L79 (*synth, ir*)

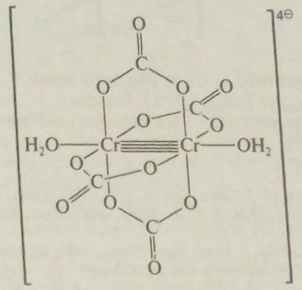
$C_4H_4CrO_{10}^{\ominus}$ IC-003925
Diaquadioxalatochromate(*III*)(1−)
Diaquabis[ethanedioato(2−)-O,O′]chromate(III)(*1−*), *11CI, 10CI, 9CI*
[15226-58-1]



cis-form

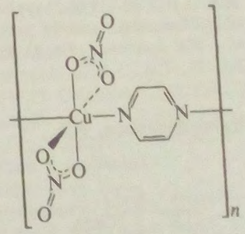
M 264.0 (ion)
Cr in an approx. octahedral arrangement; *cis* and *trans* forms are in equilm. in soln. Many salts known.
cis-form [15489-30-2]
Major isomer in aq. soln. Red-violet in aq. soln., dichroic (red-blue) in conc. soln.
K salt: [16483-17-3].
Synth. from $K_2[Cr_2O_7]$ and oxalic acid dihydrate. Deep purple cryst. + $2H_2O$. More sol. than *trans*-K salt.
trans-form [18954-99-9]
Red in aq. soln.
K salt: [14639-33-9].
Monoclinic, hard dark red or pink cryst.
[14242-38-7, 14652-48-3, 22289-32-3]
van Niekerk, J.N. *et al, Acta Crystallogr.*, 1951, **4**, 35 (*cryst struct*)
Inorg. Synth., 1977, **17**, 147 (*synth*)
Huchital, D.H. *et al, Inorg. Chim. Acta*, 1984, **95**, 127 (*isom*)
Samikkannu, S. *et al, Indian J. Chem., Sect. A*, 1986, **25**, 760 (*oxidation*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 870 (*rev*)

$C_4H_4Cr_2O_{14}^{4\ominus}$ IC-003926
Diaquatetrakis[μ-[carbonato(2−)-*O*:*O*′]]dichromate(*II*)(4−), 11CI, 10CI, 9CI
Diaquatetra-μ-carbonatodichromate(II)(4−). *Tetra-μ-carbonatodichromium*(II) *dihydrate. Tetra-μ-carbonatobis[aquachromium*(II)]
[22473-81-0]



M 380.0 (ion)
Quadruple Cr—Cr bond.
Di-Mg salt, tetrahydrate: [39912-32-8].
Air-stable cryst. Cr—Cr 222 pm.
Tetra-NH_4 salt, hydrate: [31276-88-7].
Bright yellow powder or pale brown cryst. (silica gel medium). Cr—Cr 221.4 pm.
[66197-71-5]
Ouahes, R. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **267**, 1325; 1973, **276**, 281 (*ir, cryst struct*)
Ouahes, R. *et al, Rev. Chim. Minér.*, 1970, **7**, 855.
Cotton, F.A. *et al, Inorg. Chem.*, 1978, **17**, 2004; 1982, **21**, 2675 (*cryst struct, synth*)

$C_4H_4CuN_4O_6$ IC-003927
Bis(nitrato-*O*)(pyrazine-*N*¹)copper(*II*), 11CI, 10CI, 9CI
Dinitrato(pyrazine)copper(II), *8CI. Cupric nitrate pyrazine complex*
[28209-64-5]



M 267.6
Chain struct. Obt. by evaporation of an aq. soln. of cupric nitrate and pyrazine. Cryst.
Santoro, A. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 979 (*cryst struct*)
Kokoszka, G.F. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 3229 (*esr*)

Hatfield, W.E. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 4081 (*magnetism*)
Stoklosa, H.J. *et al*, *Inorg. Chem.*, 1975, **14**, 2378 (*synth, uv, ir*)
Boyd, P.D.W. *et al*, *Inorg. Chem.*, 1980, **19**, 3547 (*magnetism*)

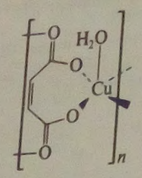
IC-003928

$C_4H_4CuO_5$

Aqua[2-butenedioato(2−)-*O,O'*]copper, 10CI

Aqua(maleato)copper. Copper(II) *maleate hydrate*

[21996-33-8]



M 195.6

Square pyramidal at Cu in polymeric struct. V. light blue cryst. μ_{eff} = 2.00μ_B (298K). See also Tetraaquacopper(2+) bis(hydrogen *cis*-2-butenedioate), IC-006039.

[34755-10-7]

Prout, C.K. *et al*, *J. Chem. Soc. A*, 1971, 3342 (*synth, cryst struct*)
Sathyanarayana, D.N. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **385**, 329 (*ir, uv*)
Mishra, H.C. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 605 (*synth, magnetism, ir, thermal props, cryst struct*)

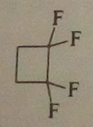
IC-003929

$C_4H_4F_4$

1,1,2,2-Tetrafluorocyclobutane

Fluorocarbon C-354

[374-12-9]



M 128.0

Synth. by the cycloaddition reaction of CF_2=CF_2 and CH_2=CH_2. Working fluid for heat pumps, aerosol spray propellant. d_4^{25} 1.275. Bp 50°. n_D^{20} 1.3038, n_D^{25} 1.3046.

▷ Potentially explosive synth.

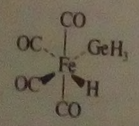
Coffman, D.D. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 490 (*synth, haz*)
Durig, J.R. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 649 (*ir, raman*)
Ravishankata, A.R. *et al*, *J. Phys. Chem.*, 1975, **79**, 876 (*ms*)
Rosmer, R.M. *et al*, *Thermochim. Acta*, 1975, **13**, 84 (*props*)
Durig, J.R. *et al*, *J. Mol. Spectrosc.*, 1976, **63**, 459 (*microwave*)

IC-003930

$C_4H_4FeGeO_4$

Tetracarbonylgermylhydroiron, 9CI

[61139-16-0]



M 244.5

Colourless volatile liq. Mp °*ca.* −30. V.p. 3.5 mm at 22°. Monomeric. Dec. in 3 days at r.t. in a sealed tube.

Stobart, S.R., *J. Chem. Soc., Dalton Trans.*, 1972, 2442 (*synth, ir, pmr*)
Gerlach, R.F. *et al*, *J. Organomet. Chem.*, 1976, **118**, C23 (*synth*)

IC-003931

$C_4H_4FeO_6$

Diaqua[3,4-dihydroxy-3-cyclobutene-1,2-dionato(2−)-*O*^{3},*O*^{4}]iron, 9CI

Iron(II) *squarate dihydrate*

[33679-04-8]

$Fe(C_4O_4)(H_2O)_2$

M 203.9

Polymeric struct. with Fe(*II*) ions at centres of edges of cube with squarate ions in cube faces. Octahedral coordn. at Fe. Synth. from aq. $K_2C_4O_4$ + $FeCl_2.6H_2O$. Yellow-green solid; relatively stable towards oxidn. if stored dry. Paramagnetic from 1.3 to 300K. Ni(*II*) analogue also reported.

West, R. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 2589 (*synth*)
Habenschuss, M. *et al*, *J. Chem. Phys.*, 1974, **61**, 852 (*struct, magnetism*)
Long, G., *Inorg. Chem.*, 1978, **17**, 2702 (*mössbauer, uv-vis, ir, magnetism, struct*)
Wrobleski, J.T. *et al*, *Inorg. Chem.*, 1979, **18**, 2738 (*magnetism, mössbauer*)

IC-003932

$C_4H_4HgO_6$

Mercury tartrate

Mercury 2,3-dihydroxybutanedioate. 2,3-Dihydroxybutanedioic acid mercury salt (1:1). Tartaric acid, mercury salt (1:1)

[22438-98-8]

Hg(OOCCHOHCHOHCOO)

M 348.6

Full struct. not detd.; presumably polymeric. Used in asym. oxymercuration and in asym. openings of epoxides. Cryst. Sol. H_2O (0.06 g per 100 cm^3). Mp >200°.

[34019-79-9]

Tikhonov, A.C., *Zh. Neorg. Khim.*, 1958, **3**, 296 (*synth*)
Kubecova, K. *et al*, *Collect. Czech. Chem. Commun.*, 1969, **34**, 1141 (*synth, ir, powder struct*)
Frei, V. *et al*, *Collect. Czech. Chem. Commun.*, 1969, **34**, 1304 (*thermal anal*)
Carlson, R.M. *et al*, *Tetrahedron Lett.*, 1971, 3661 (*synth*)
Sugita, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 1945 (*synth*)
Yamashita, H., *Bull. Chem. Soc. Jpn.*, 1988, **61**, 1213 (*synth*)

IC-003933

$C_4H_4MnO_6$

Manganese(*II*) tartrate

[36680-83-8]

Mn[OOCCHOHCHOHCOO]

M 203.0

Obt. using (*R,R*)-tartaric acid. Synth. by heating corresp. dihydrate at 135-150°. μ_{ett} = 5.93 (297K).

Dihydrate: see *Diaqua[2,3-dihydroxybutanedioato(2−)-O*^{1},*O*^{2}*]manganese*(II), *IC-004081*

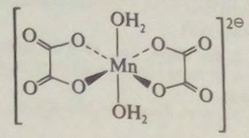
Ranade, A.A. *et al*, *Indian J. Chem.*, 1966, **4**, 42 (*magnetism*)
Kubecová, K. *et al*, *Collect. Czech. Chem. Commun.*, 1969, **34**, 1141 (*synth, powder struct, ir*)
Carillo, A. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 912 (*ir*)
Pleua, E. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1973, **69**, 355 (*esr*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 169 (*rev, bibl*)

$C_4H_4MnO_{10}^{2\ominus}$

IC-003934

Diaquabis(oxalato)manganate(*II*)(2−)

Diaquabis[ethanedioato(2−)-O,O']manganate(II)(2−)



M 267.0 (ion)

Synth. from $MnC_2O_4.2H_2O$ and $C_2O_4^{2\ominus}$ in H_2O.

Di-K salt: [20982-86-9].
Cryst.

[29335-59-9, 53199-39-6]

Graddon, D.P., *J. Inorg. Nucl. Chem.*, 1956, **3**, 308 (*uv*)
Asmussen, R.W. *et al*, *Acta Chem. Scand.*, 1957, **11**, 1331 (*magnetism*)
Schulz, H., *Acta Crystallogr., Sect. B*, 1974, **30**, 1318 (*cryst struct, ir*)
Yoshino, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 2787 (*ir*)
Nagase, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 868 (*synth, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 104 (*rev, bibl*)

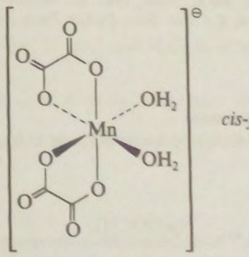
IC-003935

$C_4H_4MnO_{10}^{\ominus}$

Diaquabis(oxalato)manganate(*III*)(1−)

Diaquabis[ethanedioato(2−)-O,O']manganate(1−), 11CI

[16244-66-9]



cis-form

M 267.0 (ion)

Both *cis* and *trans*-forms known. Dissolving either isomer in H_2O gives a yellow soln. in which the *trans* isomer predominates. The solns. dec. easily, even in the dark, to give MnC_2O_4, CO_2 and $C_2O_4^{2\ominus}$.

cis-form

K salt: [36870-03-8].
Synth. from powdered $KMnO_4$ and $H_2C_2O_4.2H_2O$ in EtOH at 0° followed by addition of KOH in EtOH to the filtered brown soln. Yellow-green ppt.

K salt, trihydrate: [34032-52-5].
Synth. from stoichiometric amounts of powdered $KMnO_4$ and $H_2C_2O_4$ in H_2O at 1°. Green cryst. (95% EtOH).

trans-form

K salt, trihydrate: Synth. as for the *cis*-complex but using 1% excess $H_2C_2O_4$ and less EtOH to ppt. complex. Golden yellow cryst.

[56297-95-1]

Cartledge, G.H. *et al*, *J. Am. Chem. Soc.*, 1936, **58**, 2061, 2065 (*synth*)
Oncescu, T. *et al*, *Rev. Roum. Chim.*, 1963, **8**, 73 (*ir*)
Dingle, R., *Acta Chem. Scand.*, 1966, **20**, 33 (*uv*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1593 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 108 (*rev, bibl*)

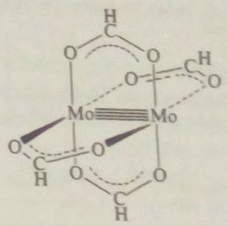
IC-003936

$C_4H_4Mo_2O_8$

Tetrakis[μ-(formato-*O*:*O'*)]dimolybdenum, 9CI

Tetra-μ-formatodimolybdenum(II)

[51329-49-8]



M 371.9

Three polymorphs known. Prepd. from $Mo(CO)_6$ + formic acid in refluxing diglyme. Yellow needles. Air-sensitive especially when moist.

Hochberg, E. *et al*, *Inorg. Chem.*, 1974, **13**, 1824 (*ms*)
Cotton, F.A. *et al*, *J. Coord. Chem.*, 1976, **5**, 217 (*synth, cryst struct*)
Mayer, J.M. *et al*, *Inorg. Chem.*, 1983, **22**, 2774 (*synth*)
Manning, M.C. *et al*, *J. Phys. Chem.*, 1983, **87**, 3083 (*uv, raman*)
Robbins, G.A. *et al*, *Inorg. Chem.*, 1984, **23**, 2086 (*cryst struct, polymorphs*)

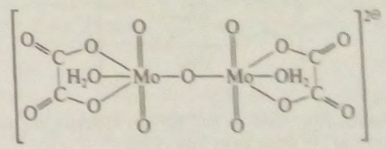
IC-003937

$C_4H_4Mo_2O_{15}^{2\ominus}$

Diaquabis(oxalato)-μ-oxotetraoxodimolybdate(*VI*)(2−)

Diaquabis[ethanedioato(2−)-O,O']-μ-oxotetraoxodimolybdate(2−), 10CI

[63312-76-5]



M 483.9 (ion)

Synth. by treatment of $[Mo_2O_4(C_2O_4)_2(OH)_2]^{2\ominus}$ with $HCrO_4^{\ominus}$. Forms a distorted octahedra.

Di-Na salt: [99635-90-2].
Synth. by treatment of $H_2C_2O_4.2H_2O$ with MoO_3 in presence of NaCl. White cryst. (H_2O). Diamagnetic.

Di-K salt: [22827-21-0].
Synth. by treatment of $H_2C_2O_4.2H_2O$ and $H_2MoO_4.H_2O$ with KCl in H_2O. Colourless cryst. (H_2O). Actually a binuclear complex of Mo(*VI*), and not of Mo(*V*) as in $C_4H_4K_2Mo_2O_{14}$, as originally thought. Shows photochromism in visible light.

Di-Rb salt: [63312-74-3].
Synth. by treatment of $H_2C_2O_4.2H_2O$ with MoO_3 in presence of RbCl. White cryst. (H_2O). Diamagnetic.

Sr salt: [95528-09-9].
Synth. by treatment of $H_2C_2O_4.2H_2O$ with MoO_3 in presence of $SrCl_2$. White cryst. + $2H_2O$ (H_2O). Diamagnetic.

Ba salt: [96342-50-6].
Synth. by treatment of $H_2C_2O_4.2H_2O$ with MoO_3 in presence of $BaCl_2$. White cryst. + $2H_2O$ (H_2O). Diamagnetic.

Di-NH_4 salt: [77115-78-7].
Synth. by treatment of $H_2C_2O_4.2H_2O$ and $H_2MoO_4.H_2O$ with NH_4Cl in H_2O. Shows photochromism in visible light.

Cotton, F.A. *et al, Inorg. Chem.*, 1964, **3**, 1603 (*deriv*)
Knobler, C. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 248 (*deriv*)
Mentzen, B. *et al, J. Photochem.*, 1981, **15**, 169 (*derivs*)
Goel, S.P. *et al, Thermochim. Acta*, 1985, **84**, 87; 1985, **95**, 295 (*deriv*)
Goel, S.P. *et al, J. Therm. Anal.*, 1986, **31**, 369 (*deriv*)
Kwon, C.Y. *et al, Taehan Hwahakhoe Chi*, 1986, **30**, 231; *CA*, **104**, 213944p (*synth*)

$C_4H_4N_4NiO_2S_4^{2\ominus}$ IC-003938

Diaquatetrakis(thiocyanato-*N*)nickelate(2−)
Diaquatetraisothiocyanatonickelate(II)(*2−*), *8CI*
[15556-24-8]

$[Ni(OH_2)_2(NCS)_4]^{2\ominus}$

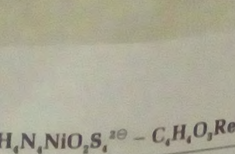
M 327.0 (ion)
Characterisation is uncertain. Assumed present in conc. aq. solns. containing $Ni^{2\oplus}$ and $NCS^{\ominus}$. Ni descr. as possessing octahedral geometry.

Hg salt:
$C_4H_4HgN_4NiO_2S_4$ M 527.6
No phys. props. reported. Formulated as $NiHg(SCN)_4.2H_2O$.

Poraj-Košic, M.A., *Acta Crystallogr.*, 1963, **16**, A42 (*Hg deriv, struct*)
Jordan, R.B. *et al, Inorg. Chem.*, 1965, **5**, 1906.

$C_4H_4NbO_{11}^{\ominus}$ IC-003939

Diaquabis(oxalato)oxoniobate(*V*)(1−)
Diaquabis[ethanedioato(2−)-O,O′]oxoniobate(V)(*1−*), *10CI*



M 320.9 (ion)
Pentagonal bipyramid. K and Rb salt hydrates are also known as are some anhydrous salts.

NH_4 salt: [58917-07-0].
Synth. by fusing Nb_2O_5 and K pyrosulfate, digesting with NH_4OH/oxalic acid and redissolving the precipitate in oxalic acid and NH_4Cl. Colourless solid $+3H_2O$ (H_2O).

Cs salt: [41673-15-8].
Synth. like the NH_4 salt but adding CsCl. Colourless solid $+ 2H_2O$ (H_2O).

Kojić-Prodić, B. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 864 (*cryst struct*)
Brnicevic, N. *et al, J. Less-Common Met.*, 1976, **45**, 45 (*synth*)
Galesic, N. *et al, J. Less-Common Met.*, 1977, **51**, 259 (*nd*)

$C_4H_4NiO_{10}^{2\ominus}$ IC-003940

Disquadioxalatonickelate(*II*)(2−), 8CI
Diaquabis(1,2-ethanedioato-O,O′)nickelate(II)(*2−*)
[15608-99-8]

$[Ni(OH_2)_2(C_2O_4)_2]^{2\ominus}$

M 270.7 (ion)
Probably octahedral with *trans* H_2O. Paramagnetic.

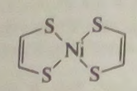
Di-K salt: [25360-78-5].
$C_4H_4K_2NiO_{10}$ M 348.9
Di-K salt, tetrahydrate: [19567-07-0].
Green solid. Can be considered as hexahydrate of K salt of $[Ni(C_2O_4)_2]^{2\ominus}$.

[20710-60-5, 24899-51-2]

Brinkley, S.R., *J. Am. Chem. Soc.*, 1939, **61**, 965 (*synth*)
Morrison, J.T. *et al, Inorg. Chim. Acta*, 1969, **3**, 463 (*synth, magnetism, uv*)
van Kraligen, C.G. *et al, Transition Met. Chem.*, 1978, **3**, 90.

$C_4H_4NiS_4$ IC-003941

Bis[1,2-ethenedithiolato(2−)]nickel, 8CI
Bis(ethylenedithiolato)nickel
[19042-52-5]



M 239.0
Simplest example of Ni dithiolene complexes. Forms stacked struct. with some org. mols, showing 1-dimensional electric conductance, periodically distorted. Brilliant violet needles. Sol. common org. solvs.

Compd. with napthaceno[5,6-cd:11,12-c′d′]bis[1,2]dithiole(5:6): [63288-57-3].
Props. not recorded.

[64685-31-0]

Hoyer, E. *et al, Chem. Ind. (London)*, 1965, 652 (*synth*)
Interrante, L.V. *et al, Ann. N.Y. Acad. Sci.*, 1978, **313**, 407 (*deriv*)
Herman, Z.S. *et al, Inorg. Chem.*, 1982, **21**, 46 (*uv*)
Ahmad, M.M. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 165 (*uv, props*)

$C_4H_4NpO_8$ IC-003942

Neptunium(*IV*) formate
Tetrakis(formato-O,O′)neptunium(IV), *9CI. Neptunium tetraformate*
[59954-48-2]

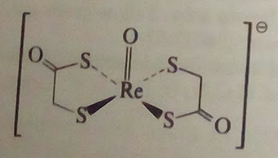
$Np(OOCH)_4$

M 417.1
Contains 10-coordinate Np. Brown solid.

Hauck, J., *Inorg. Nucl. Chem. Lett.*, 1976, **12**, 617 (*cryst struct*)
Greis, O. *et al, Z. Anorg. Allg. Chem.*, 1977, **433**, 111 (*synth, ir*)

$C_4H_4O_3ReS_4^{\ominus}$ IC-003943

Bis(mercaptothioacetato)oxorhenate(*V*)
Bis[mercaptoethanethioato(2−)-S,S′]oxorhenate(V)(*1−*), *10CI*



trans-form

M 414.5 (ion)
Square pyramidal; exists as *cis*/*trans* mixt.

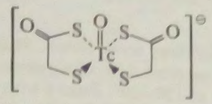
Tetrabutylammonium salt: [73396-12-0].
Synth. from $Bu_4N[ReOBr_4]$ and commercial thioglycolic acid in MeOH aq. Orange needles. Mp 129-132°.

[73465-08-4]

Davison, A. *et al, Inorg. Chem.*, 1980, **19**, 1988 (*synth, ir, uv, magnetism, electrochem*)

$C_4H_4O_5S_4Tc^{\ominus}$ IC-003944

Bis(mercaptothioacetato)oxotechnetate(*V*)(1−)
Oxobis(thiomercaptoacetato)technetate(V)(*1−*).
Bis[mercaptoethanethioato(2−)-S,S′]oxotechnetate(*1−*), *10CI*



cis-form

M 327.2 (ion)
cis (Less soluble) and *trans* isomers claimed. Synth. from $TcO_4^{\ominus}$ or $TcOCl_4^{\ominus}$ and commercial thioglycolic acid or thiomercaptoacetic acid in MeOH.

Tetrabutylammonium salt: [72043-36-8].
Orange-brown solid (aq. Me_2CO).

[73465-10-8]

De Pamphilis, B.V. *et al, J. Am. Chem. Soc.*, 1978, **100**, 5570 (*synth, cryst struct*)
De Pamphilis, B.V. *et al, J. Labelled Compd. Radiopharm.*, 1979, **16**, 26 (*synth, cryst struct*)
Davison, A. *et al, Inorg. Chem.*, 1980, **19**, 1988 (*synth, pmr, ir, uv, magnetism, electrochem*)

$C_4H_4O_5Pb$ IC-003945

Hydroxybutanedioatolead(*II*)
Lead malate. Lead(II) *hydroxybutanedioate*
[816-68-2]

$Pb(OOCCHOHCH_2COO)$

M 339.2
White powder. Sl. sol. cold H_2O; v. sl. sol. EtOH.
▷ EJ9971000.

Auerbach, F. *et al, Z. Anorg. Allg. Chem.*, 1925, **147**, 68 (*props, synth*)
Shevchenko, L.L. *et al, Zh. Prikl. Spektrosk.*, 1976, **25**, 927 (*ir, pmr*)

$C_4H_4O_5S_2Tc^{\ominus}$ IC-003946

Bis(mercaptoacetato)oxotechnetate(*V*)(1−)
Oxobis(thioglycolato)technetate(V)(*1−*)

$[TcO(SCH_2COO)_2]^{\ominus}$

M 295.1 (ion)
Early reports of Tc-mercaptoacetate complexes are dubious; commercial thioglycolic acid contains thiomercaptoacetic acid impurity which preferentially complexes technetium (see Bis(mercaptothioacetato) oxotechnetate(*V*)(1−), IC-003944).

Miller, F.J. *et al, Anal. Chem.*, 1960, **32**, 1429.
De Pamphilis, B.V. *et al, J. Am. Chem. Soc.*, 1978, **100**, 5570.
Davison, A. *et al, Inorg. Chem.*, 1980, **19**, 1988.

$C_4H_4O_6Pb$ IC-003947

Lead(*II*) tartrate
2,3-Dihydroxybutanedioic acid, lead(2+) *salt* (*1:1*), *9CI*
[815-84-9]

$Pb[OOCCHOHCHOHCOO]$

M 355.2
R,R-tartaric acid presumed. Synth. from $Pb(NO_3)_2$ + aq. alkaline sodium tartrate. White solid. Dec. in discrete stages on heating at 240-385°, eventually to PbO.
▷ OG4800000.

Kubecova, K. *et al, Collect. Czech. Chem. Commun.*, 1969, **34**, 1141 (*synth, ir, powder struct*)
Frei, V. *et al, Collect. Czech. Chem. Commun.*, 1969, **34**, 1304 (*thermal anal*)
Bottari, E. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 921 (*soln studies*)
Smolik, M. *et al, Zesz. Nauk. Politech. Slask. Chem.*, 1975, **78**, 43 (*dec*)

$C_4H_4O_6Sn$ IC-003948

Tin(*II*) tartrate
2,3-Dihydroxybutanedioic acid, tin(2+) *salt*, *9CI*
[815-85-0]

$[OOCCH(OH)CH(OH)COO]Sn$

M 266.7
Used in radiodiagnostic formulations contg. ^{99m}Tc.

Zolotukhin, I., *J. Gen. Chem. USSR (Engl. Transl.)*, 1949, **19**, 973 (*synth*)
Lees, J. *et al, Phys. Lett.*, 1965, 186 (*mössbauer*)
Yamashita, H., *Bull. Chem. Soc. Jpn.*, 1988, **61**, 1213 (*synth*)

$C_4H_4O_6Zn$ IC-003949

Zinc *R,R*-tartrate
Zinc 2,3-dihydroxybutanedioate. 2,3-Dihydroxybutanedioic acid zinc salt (*1:1*). *Tartaric acid, zinc salt* (*1:1*)
[551-64-4]

$Zn(OOCCHOHCHOHCOO)$

M 213.4
Older literature cites a dihydrate; the cryst. struct. of a 2:5 hydrate however has been determined. Obt. by heating hydrate(s) at 150°. Catalyst for ring-opening of epoxides; smoke inhibitor; used in dentifrice and pvc; used with cyanoacrylate adhesives. Solid. Sol. H_2O (1.9 g per 100 cm^3). Dec. at 310-400° to ZnO.

Dihydrate: [22570-08-7].
Solid. Dehydrates at 150°/1 mm for 5h.

2.5 hydrate: [96242-80-7]. *Di-μ-(+)-tartratobis[aquazinc*(II)*] trihydrate. Diaquabis[μ-[2,3-dihydroxybutanedioato(2−)-O^1,O^2,O^3,O^4]]dizinc trihydrate*
Cryst.

Pickering, S.U., *J. Chem. Soc.*, 1916, **109**, 235.
Frei, V. *et al, Collect. Czech. Chem. Commun.*, 1964, **29**, 1418; 1965, **30**, 777 (*ir, synth, thermal anal, dihydrate*)
Swinarski, A. *et al, Collect. Czech. Chem. Commun.*, 1966, **31**, 4333 (*stability const*)
Kubecova, K. *et al, Collect. Czech. Chem. Commun.*, 1969, **34**, 1141 (*synth, ir, powder struct, dihydrate*)
Carillo, A. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1972, **274**, 912 (*ir, uv-vis*)
Templeton, L.K. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 363 (*cryst struct, 2.5 hydrate*)
Yamashita, H., *Bull. Chem. Soc. Jpn.*, 1988, **61**, 1213 (*synth*)

$C_4H_4O_7V^{\ominus}$ IC-003950

Bis[hydroxyacetato(2−)-O^1,O^2]oxovanadate(*V*)(1−), 11CI

$[(OCH_2COO)_2VO]^{\ominus}$

M 215.0 (ion)
Struct. unknown.

NH_4 salt: [83299-69-8].
Synth. by adding NH_4VO_3 to aq. HOAc and hydrazine, followed by hydroxyacetic acid and NH_4OH to adjust pH to 7.5. Shows broad antimicrobial action. Blue solid ($EtOH/Me_2CO$). Sol. H_2O. Mp 252-253°.

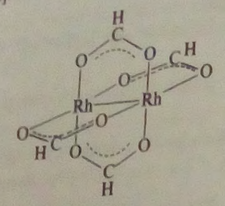
Datta, S. *et al, Agents Actions*, 1982, **12**, 543; *CA*, **97**, 159388g (*pharmacol*)
Dey, K. *et al, Indian J. Chem., Sect. A*, 1983, **22**, 580 (*synth, ir, uv-vis, bioassay*)

IC-003951

$C_4H_4O_8Rh_2$

Tetrakis[μ-(formato-*O*:*O*′)]dirhodium(*II*)

[33773-07-8]



M 385.8
Prob. has $M_2(RCO_2)_4$ dinuclear struct. Model for theoretical studies of $Rh_2(O_2CR)_4$ compds.

Monohydrate: [15005-99-9].
Dark green cryst. Sol. hot H_2O.

Dihydrate: [33700-44-6]. *Diaquatetrakis[μ-(formato-O:O′)]dirhodium*(II)
$C_4H_8O_{10}Rh_2$ M 421.9
Model for theoretical studies of $Rh_2(O_2CR)_4L_2$ complexes. Coordinated H_2O's occupy axial positions in dinuclear struct.

Bis-PH_3 complex: [77965-51-6]. *Tetrakis[μ-formato-O:O′]bis(phosphine)dirhodium, 10CI*
$C_4H_{10}O_8P_2Rh_2$ M 453.8
Prototype: not prepd., but used as model for molecular orbital calculations on $[Rh_2(O_2CR)_4L_2]$ complexes.

Chernyaev, I.I. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1966, **11**, 1383 (*synth*)
Norman, J.G. *et al, J. Am. Chem. Soc.*, 1978, **100**, 791 (*theory, dihydrate*)
Mazo, G.Y. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1855 (*ir, dihydrate*)
Bernstein, B.E. *et al, Inorg. Chem.*, 1981, **20**, 3042 (*theory*)

IC-003952

$C_4H_4O_8Th$

Thorium(*IV*) formate

Tetrakis(formato-O,O′)thorium(IV)

[59954-45-9]

$Th(OOCH)_4$

M 412.1
10-Coord., isomorphous with Np analogue. White cryst. Sol. H_2O; sl. sol. MeOH. Dec. to ThO_2 >290°.

Trihydrate: White cryst. Sol. H_2O. 10-Coord. bicapped antiprismatic struct. Forms anhydrous salt on heating.

Golovnya, V.A. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1963, **8**, 1290.
Claudel, B. *et al, Bull. Soc. Chim. Fr.*, 1966, 1547 (*struct*)
Arutyunyan, E.G. *et al, Zh. Strukt. Khim.*, 1966, **7**, 471.
Mentzen, B., *Rev. Chim. Miner.*, 1969, **6**, 713 (*struct*)
Molodkhin, B.K. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 1692 (*hydrate, cryst struct*)
Mentzen, B., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **276**, 229.
Hauck, J., *Inorg. Nucl. Chem. Lett.*, 1976, **12**, 617 (*cryst struct*)
Greis, O. *et al, Z. Anorg. Allg. Chem.*, 1977, **433**, 111 (*synth, ir*)

IC-003953

$C_4H_4O_8U$

Uranium(*IV*) formate

Tetrakis(formato-O,O′)uranium(IV)

[59954-47-1]

$U(OOCH)_4$

M 418.1
10-Coordinate. Exists in three cryst. forms. Moisture-sensitive dark green or olive monoclinic cryst. Dec. to $UO_2(HCOO)_2$ in air at 120-220°. Reacts with NH_3, CH_3NH_2 with oxidation to U(*VI*) formate complexes.

Rosenheim, A. *et al, Z. Anorg. Allg. Chem.*, 1932, **43**, 206 (*synth*)
Bressat, R. *et al, Bull. Soc. Chim. Fr.*, 1968, **12**, 4807 (*synth*)
Bressat, R. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **266**, 1260 (*dta, tga*)
Buttres, R. *et al, J. Chem. Soc. A*, 1968, 1272.
Mentzen, B., *Rev. Chim. Minér.*, 1969, **6**, 713 (*struct*)
Hauck, J., *Inorg. Nucl. Chem. Lett.*, 1976, **12**, 617 (*cryst struct*)
Greis, O. *et al, Z. Anorg. Allg. Chem.*, 1977, **433**, 111 (*synth, ir*)
Spitsyn, V.I. *et al, Zh. Neorg. Khim.*, 1982, **27**, 849; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 476 (*reactions*)

IC-003954

$C_4H_4O_9V^{2\ominus}$

Tetrakis(formato-*O*)oxovanadate(*IV*)(2−), 11CI

(*μ-Formato*)*triformatooxovanadate*(IV)(*2*−)

$[VO(OOCH)_4]^{2\ominus}$

M 247.0 (ion)
Octahedral polymer with formate groups bridging *cis*-positions.

Di-K salt: [103572-85-6].
Synth. by dissolving K_2CO_3 and VO(formate)$_2$ in formic acid/MeOH then adding excess formic acid/MeOH. Blue solid. Paramagnetic; $\mu_{eff} = 1.79\mu_B$ (298K).

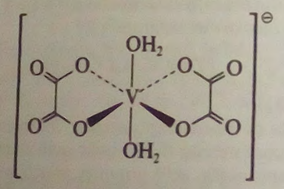
Gilson, T.R. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 895 (*synth, cryst struct, esr, magnetism*)

IC-003955

$C_4H_4O_{10}V^{\ominus}$

Diaquabis(oxalato)vanadate(*III*)(1−)

Diaquabis[ethanedioato(2−)-O,O′]vanadate(III)(*1*−), *11CI*



M 263.0 (ion)
Octahedral.

***trans*-form**

Cs salt: [97385-43-8].
Synth. from $VCl_3.6H_2O$ and oxalic acid in H_2O followed by addn. of CsCl. Red-purple solid + $4H_2O$ (H_2O).

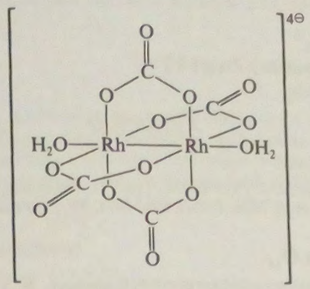
$MeNH_3$ salt: [97107-09-0].
Synth. as for the Cs salt using $[MeNH_3]Cl$. Red-purple solid + $4.5H_2O$ (H_2O).

Grey, I.E. *et al, Acta Crystallogr., Sect. C*, 1985, **41**, 681 (*synth, cryst struct*)

IC-003956

$C_4H_4O_{14}Rh_2^{4\ominus}$

Diaquatetrakis(μ-carbonato)dirhodate(*II*)(4−), 10CI



M 481.8 (ion)
Carbonate analogue of $M_2(O_2CR)_4$ struct.

Tetra-Cs salt: [72207-19-3].
Dark blue cryst. + $6H_2O$.

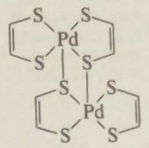
Cotton, F.A. *et al, Inorg. Chem.*, 1980, **19**, 320 (*synth, cryst struct*)

IC-003957

$C_4H_4PdS_4$

Bis(1,2-ethenedithiolato-*S*,*S*′)palladium

Bis(1,2-dithiolatoethene)palladium



dimer

M 286.7
Prepd. by I_2 oxidation of $[PdS_4C_4H_4]^{\ominus}$. Cryst. (CS_2).

Dimer: [35163-38-3]. *Tetrakis[1,2-ethenedithiolato(2−)-S,S′]dipalladium, 9CI*
$C_8H_8Pd_2S_8$ M 573.5

Browall, K.W. *et al, Inorg. Chem.*, 1972, **11**, 1800 (*synth, cryst struct*)

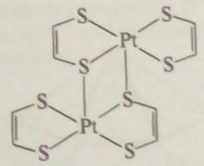
IC-003958

$C_4H_4PtS_4$

Bis(1,2-ethenedithiolato-*S*,*S*′)platinum, 9CI

Bis(1,2-dithiolatoethene)platinum

[35163-39-4]



M 375.4
Dimeric struct. with PtS_4 square planar units linked by Pt—Pt interaction of 277 pm.

Dimer: Tetrakis(1,2-ethenedithiolato-S,S′)diplatinum
$C_8H_8Pt_2S_8$ M 750.8
Black solid. Spar. sol. $CHCl_3$, CS_2, C_6H_6. One-dimensional electrical conductor.

[66906-50-1]

Browall, K.W. *et al, Inorg. Chem.*, 1972, **11**, 1800 (*synth, cryst struct, cond*)

IC-003959

$C_4H_5AuO_4S$

Mercaptobutanedioato(1−)gold, 9CI

Gold thiomalate. [(*1,2-Dicarboxyethyl*)*thio*]*gold. Aurothiomalic acid*

$HOOCCH_2CH(SAu)COOH$

M 346.1

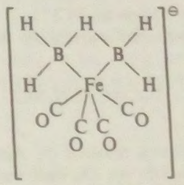
Di-Na salt: [12244-57-4]. *Gold sodium thiomalate. Sodium aurothiomalate. Myochrysine. Myocrisin. Tauredon*
$C_4H_3AuNa_2O_4S$ M 390.0
Antirheumatic drug. Yellowish-white powder. Sol. H_2O, insol. EtOH, Et_2O.
▷ MD5435000.

Merck Index, 9th Ed., 1976, No. 4365.
Sadler, P.J., *Struct. Bonding* (*Berlin*), 1976, **29**, 171 (*rev*)
Shaw, C.F. *et al, Inorg. Perspect. Biol. Med.*, 1979, **2**, 287 (*rev*)
Brown, D.H. *et al, Chem. Soc. Rev.*, 1980, **9**, 217 (*rev*)
Brown, K. *et al, J. Am. Chem. Soc.*, 1981, **103**, 4943 (*mössbauer*)

IC-003960

$C_4H_5B_2FeO_4^{\ominus}$

Tetracarbonyl[η²-pentahydrodiborato(1−)]ferrate(1−)



M 194.5 (ion)
Proposed struct. shown.

K salt: [67269-71-0].
Dark brown solid., stable at r.t. for several hours sealed under vacuum. Sol. THF.

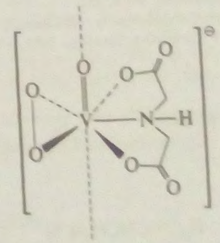
Medford, G.F. *et al, J. Am. Chem. Soc.*, 1978, **100**, 3953 (*synth, ir, pmr, B-11 nmr*)
Medford, G.F., *CA*, 1979, **90**, 80158d (*synth*)

IC-003961

$C_4H_5NO_7V^{\ominus}$

(Iminodiacetato)oxoperoxyvanadate(*V*)(1−)

[N-(*Carboxymethyl*)*glycinato*(2−)-N,O,O^{N}]*oxoperoxyvanadate*(V)(*1*−), *11CI*



M 230.0 (ion)
Pentagonal bipyramidal with the oxo and one carboxyl oxygen of a neighbouring unit in axial positions. The bridging between units is weak; V=O 237.5 pm. Has been tested for anti-tumour activity and proposed as a model for V sites in biochemical spp.

NH_4 salt: [95533-37-2].
$C_4H_8N_2O_7V$ M 248.0

Synth. from NH_4VO_3, imidodiacetic acid and H_2O_2 in aq. soln. Sol. H_2O.
K salt: [95533-36-1]
Synth. analogous to that of NH_4 salt. Sol. H_2O.
[95533-38-3]
Djordjevic, C. *et al, Inorg. Chem.*, 1985, **24**, 1281 (*synth, cryst struct*)
Djordjevic, C. *et al, J. Inorg. Biochem.*, 1985, **25**, 51 (*pharmacol*)

$C_4H_5NO_8Ru^{2\ominus}$ IC-003962

Hydroxybis[hydroxyacetato(2−)-O^1,O^2]nitrosylruthenate(2−)
Bis(glycolato)hydroxy(nitrosyl)ruthenate(2−)

$[Ru(NO)(OH)(OCH_2CO_2)_2]^{2\ominus}$

M 296.1 (ion)
pseudo-Octahedral; isomeric form unknown. Prepd. by treating $Ru(NO)Cl_3(OH_2)_2$ with $HOCH_2COOH$. Sol. H_2O.
Di-K salt: [72466-56-9].
Characterised spectroscopically. Ir ν_{NO} 1865 cm^{-1}.
Ishiyama, T. *et al, Annu. Rep. Radiat. Centre Osaka Prefect.*, 1978, **19**, 1 (*synth*)

C_4H_5NS IC-003963

3-Isothiocyanato-1-propene, 9CI
Allyl isothiocyanate. Allyl mustard oil. Mustard oil
[57-06-7]

$H_2C{=}CHCH_2NCS$

M 99.1
Chief constit. of natural mustard oil. Also found in cooked cabbage, horseradish, etc. Oil with very pungent, irritating odour. Sol. EtOH, Et_2O, C_6H_6, sl. sol. H_2O. d_4^{15} 1.015. Fp −80°. Bp 151°, Bp_{12} 44°.
▷ Highly toxic, mutagen. Autoclave reacns. between NaSCN and $H_2C{=}CHCH_2Cl$ may explode. NX8225000.
Tollens, B. *et al, Justus Liebigs Ann. Chem.*, 1870, **156**, 134 (*synth*)
Kjaer, A. *et al, Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Daxenbichler, M.E. *et al, J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)
Mathias, A., *Tetrahedron*, 1965, **21**, 1073 (*pmr*)
Food Chemicals Codex, 2nd Ed., 1972, 31 (*anal*)
Yonemoto, T. *et al, J. Magn. Reson.*, 1974, **13**, 153 (*synth*)
Mahuja, M. *et al, Indian J. Chem.*, 1976, **11**, 15 (*synth*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 469.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 351.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 171.

C_4H_5NS

3-Thiocyanato-1-propene IC-003964
Allyl thiocyanate. Allylrhodamide. Thiocyanic acid 2-propenyl ester, 9CI
[764-49-8]

$H_2C{=}CHCH_2SCN$

M 99.1
Present in seeds of *Brassica juncea*. Prod. from Sinigrin by enzymes in *Thlaspi arvense*. Pungent oil. d^{15} 1.056. Bp 161°. Rearr. on standing to 3-Isothiocyanato-1-propene, IC-003963.
▷ Highly toxic. XL2000000.

Gmelin, R. *et al, Acta Chem. Scand.*, 1959, **13**, 1474.
Kirk, L.D. *et al, J. Am. Oil Chem. Soc.*, 1964, **41**, 599.
Emerson, D.W., *J. Chem. Educ.*, 1971, **48**, 81 (*synth*)

$C_4H_6AgN_2^{\oplus}$ IC-003965

Bis(acetonitrile)silver(1+)
[55031-59-9]

$Ag(NCCH_3)_2^{\oplus}$

M 189.9 (ion)
Janz, G.J. *et al, J. Phys. Chem.*, 1967, **71**, 963 (*synth, ir*)
Roulet, R. *et al, Helv. Chim. Acta*, 1974, **57**, 2139 (*use*)

$C_4H_6As_6Cu_4O_{16}$ IC-003966

Bis(acetato)hexametaarsenitotetracopper, 8CI
Cupric acetoarsenite. Copper acetate arsenite
[12002-03-8]

$Cu_4(OAc)_2(AsO_2)_6$

M 1013.7
Insecticide; pigment; wood preservative. Emerald green cryst. Stable to air and light. Sl. sol. H_2O.
▷ Poisonous. LD_{50} (orally in female rats) 100mg kg^{-1}. GL6475000.
Avery, S., *J. Am. Chem. Soc.*, 1906, **28**, 1159 (*synth*)
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, NY, 1965-1971, **2**, 1027 (*synth*)
Gaines, T.B., *Toxicol. Appl. Pharmacol.*, 1969, **14**, 515.
Merck Index, 11th Ed., 1989, No. 2629.

$C_4H_6AuN_2^{\oplus}$ IC-003967

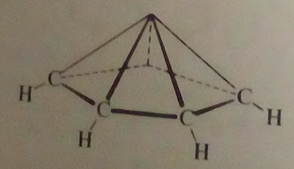
Bis(acetonitrile)gold(1+), 9CI
[44606-68-0]

$Au(NCCH_3)_2^{\oplus}$

M 279.0 (ion)
Perchlorate: [51240-11-0].
$C_4H_6AuClN_2O_4$ M 378.5
Cryst. (MeCN).
Bergerhoff, G., *Z. Anorg. Allg. Chem.*, 1964, **327**, 139 (*synth*)
Fenske, G.P. *et al, Inorg. Chem.*, 1974, **13**, 1783 (*use*)
Roulet, R. *et al, Chimia*, 1975, **29**, 346.
Johnson, P.R. *et al, J. Chem. Soc., Chem. Commun.*, 1978, 606.

$C_4H_6B_2$ IC-003968

2,3,4,5-Tetracarbahexaborane(6), 10CI
[28323-17-3]



M 75.7
nido-. Isoelectronic with B_6H_{10} without any bridge H atoms. Liq. (by dist. *in vacuo*).
Groszek, E. *et al, Inorg. Chem.*, 1971, **10**, 2770 (*synth, ir, ms, nmr*)
Miller, V.R. *et al, Inorg. Chem.*, 1972, **11**, 862 (*synth*)
Pasinski, J.P. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 928 (*microwave*)

$C_4H_6BaO_4$ IC-003969

Barium acetate
Acetic acid, barium salt, 8CI. Ethanoic acid, barium salt
[543-80-6]

$Ba(OAc)_2$

M 255.4
Synth. by addition of aq. AcOH (50%) to an aq. soln. of $Ba(OH)_2$ previously neutralised with AcOH. Commercially available. Catalyst for alkene polym. Colourless cryst. Dec. on heating with $BaCO_3$ formation. V. sol. H_2O (59 g per 100 cm^3 at 0°; 75 g per 100 cm^3 at 100°).
▷ Toxic. AF4550000.
Monohydrate: [5908-64-5].
$C_4H_8BaO_5$ M 273.4
Colourless triclinic cryst.; dec. on heating with H_2O loss (−H_2O at 150°). V. sol. H_2O (76 g per 100 cm^3 at 26°). Dehydration by $(MeO)_2CMe_2$ in MeOH gives anhyd. $Ba(OAc)_2$.
▷ Toxic.
Padmanabhan, V.M., *Proc. - Indian Acad. Sci., Sect. A*, 1953, **37**, 401; *CA*, **47**, 8515a (*raman, monohydrate*)
Herrera, J. *et al, Circ. Farm.*, 1981, **39**, 153; *CA*, 1982, **96**, 27722 (*dehydration, monohydrate*)
Baraldi, P., *Spectrochim. Acta, Part A*, 1982, **38**, 51 (*thermal dec, ir*)
Jagannathan, M.R. *et al, Indian J. Pure Appl. Phys.*, 1984, **22**, 484 (*pmr*)
Groombridge, C.J. *et al, J. Solid State Chem.*, 1985, **59**, 306 (*cmr, monohydrate*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 332C (*haz*)

$C_4H_6Br_2CrN_2$ IC-003970

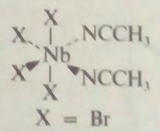
Bis(acetonitrile)dibromochromium(*II*), 8CI
Dibromobis(acetonitrile)chromium. Chromium(II) *bromide bis(acetonitrile)*

$[CrBr_2(NCCH_3)_2]_n$

M 293.9
Bromide-bridged polymer with distorted octahedral Cr. Pale blue green air-sensitive needles. Spar. sol. MeCN. μ_{eff} = 4.85μ_B (299K).
Holah, D.G. *et al, Inorg. Chem.*, 1966, **5**, 479 (*synth, uv*)
Scaife, D.E., *Aust. J. Chem.*, 1967, **20**, 845.

$C_4H_6Br_4N_2Nb$ IC-003971

Bis(acetonitrile)tetrabromoniobium(*IV*), 11CI
Tetrabromobis(methyl cyanide)niobium(IV). *Niobium*(IV) *bromide bis(acetonitrile)*
[21126-00-1]



X = Br *cis-form*

M 494.6
cis-form [22937-46-8]
Synth. by refluxing $NbBr_4$ in MeCN. Dark brown, oxygen- and moisture-sensitive solid. Paramagnetic, μ_{eff} = 1.27μ_B (300K), 1.04μ_B (80K).
Dougherty, T.A., *U.S. At. Energy Comm.*, 1967, IS-T-140; *CA*, **69**, 46920c (*cryst struct, ir*)
Fowles, G.W.A., *Inorg. Chem.*, 1969, **8**, 631 (*synth, ir, magnetism*)
Machin, D.J. *et al, J. Less-Common Met.*, 1969, **19**, 405 (*synth, uv-vis, magnetism*)

$C_4H_6CaO_4$ IC-003972

Calcium acetate
Acetic acid, calcium salt, 8CI. Ethanoic acid, calcium salt
[62-54-4]

$Ca(OAc)_2$

M 158.1
Synth. by reaction of Ac_2O with anhydrous solid $Ca(NO_3)_2$. Generation by dehydration of the dihydrate is difficult, mixtures of $Ca(OAc)_2$ with AcOH and $CaCO_3$ (or CaO) being produced. Component of lubrication greases; crosslinking agent for acrylic adhesives. Additive for polyester fibres to improve dyeability and drape; and to poly(ethylene terephthalate) films to improve friction props. Widely used as a catalyst, particularly for gasification processes. Commercially available as hydrate. Hygroscopic white powder. V. sol. H_2O (37 g per 100 cm^3 at 0°; 30 g per 100 cm^3 at 100°); spar. sol. EtOH. ΔH_f° −1479 kJ mol^{-1}. Hygroscopic. Dec. on heating to form CaO.
▷ AF7525000.
Monohydrate: [5743-26-0].
$C_4H_8CaO_5$ M 176.1
Cryst. from aq. $Ca(OAc)_2$ >84°. Colourless cryst. Dec. on heating → CaO. V. sol. (44 g per 100 cm^3 at 0°; 34 g per 100 cm^3 at 100°); spar. sol. EtOH. ΔH_f° −1772 kJ mol^{-1}.
▷ AF7875000.
Dihydrate.
$C_4H_{10}CaO_6$ M 194.1
Synth. by treatment of $Ca(OH)_2$ with Ac_2O or by neutralisation of $CaCO_3$ with glacial AcOH. Cryst. from aq. soln. of $Ca(OAc)_2$ <84°. Colourless cryst. Dec. on heating with H_2O loss (−H_2O at 84°) and ultimate formation of CaO. V. sol. H_2O (35 g per 100 cm^3 at 20°; 34 g per 100 cm^3 at 80°); spar. sol. EtOH.
Rubinshtein, A.M. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1958, **121**, 664 (*thermal dec*)
Walter-Levy, L. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1960, **250**, 3320 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 982 (*rev, bibl*)
Stoilova, D. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, **9**, 371 (*ir, monohydrate*)
Chill, J. *et al, Thermochim. Acta*, 1980, **40**, 251 (*thermal dec, tga, ms, monohydrate*)
Balimann, G.E. *et al, Philos. Trans. R. Soc. London, A*, 1981, **299**, 643 (*cmr*)
Mu, J. *et al, Thermochim. Acta*, 1981, **49**, 207 (*thermal dec*)
Jagannathan, N.R. *et al, Indian J. Pure Appl. Phys.*, 1984, **22**, 484 (*pmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 665C (*haz*)

$C_4H_6CdO_4$ IC-003973

Cadmium acetate
[543-90-8]

$Cd(OAc)_2$

M 230.5
Obt. from dihydrate at 130° *in vacuo*; or from $CdCO_3$ in AcOH. Polym. catalyst. Cryst.; dimorphic, α→β at 225°. Mp 255°. Dec. at 262° to $Cd_4O(OAc)_6$.
▷ EU9810000.

Dihydrate: [5743-04-4].
Cryst. Struct. comprises 7-coord. Cd (CdO_7) in a distorted square base trigonal capped environment; both AcO⁻ are bidentate with O of one also bridging Cd. Loses H_2O at 80° and 130°.
▷ AF730:5000.

Krishnamurti, P., *Indian J. Phys.*, 1931, **6**, 509 (*raman*)
Duval, C. *et al*, *Ann. Phys.*, 1942, **17**, 5 (*ir, a*)
Krishnamurthy, N., *Proc. Indian Acad. Sci., Sect. A*, 1963, **61**, 113 (*raman, dihydrate*)
Harrison, W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 956 (*cryst struct, dihydrate*)
Cheung, T.T.P. *et al*, *J. Magn. Reson.*, 1980, **41**, 158 (*Cd-113 nmr, solid state*)
Barahli, P., *Spectrochim. Acta, Part A*, 1982, **38**, 51 (*ir*)
Honkonen, R.S. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5488 (*Cd-113 nmr, dihydrate*)
Cammin, R. *et al*, *J. Chem. Phys.*, 1984, **81**, 343 (*cryst, solid struct*)
Ganapathy, S. *et al*, *J. Magn. Reson.*, 1984, **57**, 239 (*cryst, solid state*)
Grigor'ev, A.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1984, **29**, 376 (*thermal anal, dihydrate, ir, powder struct*)
Marchetti, V.S. *et al*, *J. Magn. Reson.*, 1987, **71**, 299 (*cryst, Cd-113 nmr, solid state*)
Tackett, J.E., *Appl. Spectrosc.*, 1989, **43**, 483 (*ir, raman*)

$C_4H_6CdO_5$ IC-003974

Diaqua[(*Z*)-2-butenedioato(2−)]cadmium(*II*)
Cadmium maleate dihydrate. Cadmium (Z)-2-butenedioate dihydrate
[26266-36-4]

$[(H_2O)_2Cd(OOCCH{=}CHCOO)]_n$

M 262.4
Dimorphic, both forms monoclinic with polymeric struct. with bridging maleates, Cd in 6-coordinate and 8-coordinate environments. Cryst. (hot H_2O) or cryst. (H_2O, 25°). Dehydrates on heating.
[52383-63-8]

Konishi, Y. *et al*, *Chem. Lett.*, 1973, 829 (*thermal anal*)
Post, M.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 674 (*synth, cryst struct*)
Hempel, A. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2215 (*synth, cryst struct*)
Mennitt, P.G. *et al*, *J. Phys. Chem.*, 1981, **85**, 2089 (*Cd-113 nmr*)
Honkonen, R.S. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5488 (*synth, Cd-113 nmr*)

$C_4H_6ClGaO_4$ IC-003975

Gallium(*III*) acetate chloride ($Ga(OAc)_2Cl$)
Gallium(III) *chloride bis(ethanoate). Diacetato(chloro) gallium*

$GaCl(OAc)_2$

M 223.2
Synth. from $GaCl_3$ + HOAc in Et_2O at 130°. Colourless prismatic moisture-sensitive cryst. Sol. MeOH, EtOH; spar. sol. Et_2O.

Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **330**, 70 (*synth, props*)

$C_4H_6ClO_5Ta$ IC-003976

Bis(acetato-*O*)chlorooxotantalum(*V*), 1Cl
[100072-32-0]

$TaO(OAc)_2Cl$

M 350.4
Polymeric: there is some evidence for bridging carboxyl groups. Synth. by adding Ac_2O to $TaCl_5$ followed by CCl_4. Brown solid. Ir $\nu_{Ta=O}$ 955 cm^{-1}.

Kapoor, R. *et al*, *Indian J. Chem., Sect. A*, 1985, **24**, 761 (*synth, ir*)

$C_4H_6Cl_3CrN_2$ IC-003977

Bis(acetonitrile)dichlorochromium(*II*), 1Cl, 1OCl, 9Cl, 8Cl
Dichlorobis(acetonitrile)chromium. Chromium(II) *chloride bis(acetonitrile)*
[15281-36-4]

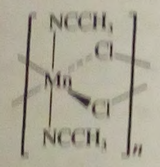
$[CrCl_2(NCCH_3)_2]_n$

M 205.0
Chloride-bridged polymer with distorted octahedral Cr. Starting material. Pale blue air-sensitive cryst. Spar. sol. MeCN; sol. EtOH. μ_{eff} = 4.81μ_B (293K).

Holah, D.G. *et al*, *Inorg. Chem.*, 1966, **5**, 479.
Inorg. Synth., 1967, **10**, 26.
Marchese, A.L. *et al*, *J. Organomet. Chem.*, 1984, **266**, 61.

$C_4H_6Cl_2MnN_2$ IC-003978

Bis(acetonitrile)dichloromanganese(*II*)
Dichlorobis(methyl cyanide)manganese(II). *Manganese*(II) *chloride bis(acetonitrile)*

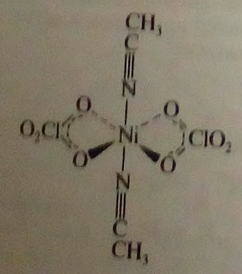


M 207.9
Octahedral Mn in polymeric chain struct. Synth. by treating a suspension of Mn in MeCN with Cl_2. Pink solid. μ_{eff} = 5.83μ_B. Bromide compd. also known.

Hathaway, B.J. *et al*, *J. Chem. Soc.*, 1964, 2400 (*synth, ir, uv, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 10 (*rev, bibl*)

$C_4H_6Cl_2N_2NiO_8$ IC-003979

Bis(acetonitrile)diperchloratonickel(*II*) 8Cl
Bis(perchlorato-O,O′)bis(acetonitrile)nickel(II). *Diperchloratobis(acetonitrile)nickel*(II). *Nickel*(II) *perchlorate bis(acetonitrile)*
[14836-72-7]

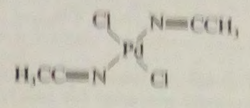


M 339.6
Pseudo-*trans*-octahedral struct. based on ir data. Standard example of bidentate perchlorate. Obtd. by thermal dec. of $Ni(NCMe)_6(ClO_4)_2$ at 75° *in vacuo*. Moisture sensitive green solid.
▷ Potentially explosive.

Wickenden, A.E. *et al*, *Inorg. Chem.*, 1965, **4**, 404 (*synth, ir, uv-vis*)

$C_4H_6Cl_2N_2Pd$ IC-003980

Bis(acetonitrile)dichloropalladium(*II*)
[14592-56-4]



M 259.4
trans-form [21264-30-2]
Widely used as a catalyst in org. synth. Yellow precipitate. Mp > 300°.
[90243-59-7]

Walton, R.A., *Spectrochim. Acta*, 1965, **21**, 1795 (*ir*)
Walton, R.A., *Can. J. Chem.*, 1968, **46**, 2347 (*ir, raman*)
Wayland, B.B. *et al*, *Inorg. Chem.*, 1969, **8**, 971 (*synth*)
Andrews, M.A. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5913 (*synth*)

$C_4H_6Cl_2N_2Pt$ IC-003981

Bis(acetonitrile)dichloroplatinum(*II*), 8Cl
Platinum(II) *chloride bis(acetonitrile). Dichlorobis(methyl cyanide)platinum*
[13869-38-0]

$PtCl_2(NCCH_3)_2$

M 348.0
Only known as *cis*-square planar form. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + MeCN. Useful intermed. for synth. of other $PtCl_2$ complexes. Oxidised by base, O_2 to 'platinblau' species. Pale yellow cryst. (MeCN). Spar. sol. most solvs.
[21264-32-4]

Hofmann, K.A. *et al*, *Ber.*, 1907, **40**, 1772 (*synth*)
Walton, R.A., *Can. J. Chem.*, 1968, **46**, 2347 (*ir, raman*)
Hartley, F.R. *et al*, *Inorg. Chem.*, 1979, **18**, 1394 (*synth*)
Laurent, M.P. *et al*, *Inorg. Chem.*, 1980, **19**, 1656 (*reactions*)
Rochon, F.D. *et al*, *Can. J. Chem.*, 1984, **62**, 860 (*cryst struct, ir, raman*)
Newkome, G.R. *et al*, *Acta Crystallogr., Sect. C*, 1986, **42**, 1643 (*struct*)

$C_4H_6Cl_2O_4Ti$ IC-003982

Bis(acetato-*O*)dichlorotitanium(*IV*), 1Cl
Titanium(IV) *diacetate dichloride*
[4644-35-3]

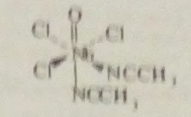
$TiCl_2(OAc)_2$

M 236.8
Synth. by reaction of $TiCl_4$ with excess HOAc, or by the reaction $TiCl_3(OAc)$ + $NOCl \rightarrow TiCl_2(OAc)_2$ + $TiCl_4.2NOCl$. Catalyst for the stereospecific polym. of butadiene and for the esterification of phthalic anhydride. White, moisture-sensitive solid.

Bolotina, L.M. *et al*, *Plast. Massy*, 1973, 13; *CA*, **79**, 147048m (*use, catalysis*)
Amaudrat, J., *Bull. Soc. Chim. Fr.*, 1975, 1579; 1977, 624 (*synth, ir*)
Rafikov, S.R. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1975, 1615; *CA*, **83**, 193805m (*use, polym*)

$C_4H_6Cl_3N_2NbO$ IC-003983

Bis(acetonitrile)trichlorooxoniobium(*V*), 9Cl
Oxotrichlorobis(methyl cyanide)niobium(V)
[56349-60-1]



M 297.3
Distorted octahedron. ONbCl angles vary between 97 and 101°. Synth. by recrystallising $NbOCl_3$ from dry MeCN. Cryst.

Chavant, C. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1828 (*synth, cryst struct*)

$C_4H_6Cl_3N_2NbS$ IC-003984

Bis(acetonitrile)trichlorothioxoniobium(*V*), 1Cl
Bis(acetonitrile)trichlorosulfidoniobium(V)
[63510-32-7]

$NbCl_3S(NCCH_3)_2$

M 313.4
Presumed octahedral at Nb. Synth. by refluxing $NbCl_3S$ in MeCN. Green solid. Sol. MeCN. Ir $\nu_{Nb=S}$ 528 cm^{-1}.

Baghlaf, A.O. *et al*, *J. Less-Common Met.*, 1977, **53**, 291 (*synth, ir*)
bin-Baba, I., *Sains Malays.*, 1983, **12**, 249 (*synth, ir, uv-vis*)

$C_4H_6Cl_3N_2NbSe$ IC-003985

Bis(acetonitrile)trichlorooxoseleniobium(*V*), 1Cl
Bis(acetonitrile)trichlorooxoselenidoniobium(V). *Niobium*(V) *trichloride selenide bis(acetonitrile)*
[92205-08-8]

$NbCl_3Se(NCCH_3)_2$

M 360.3
Presumed octahedral. Synth. by refluxing $NbCl_3Se$ in excess MeCN. Dark brown solid. Sol. MeCN.

bin-Baba, I., *Sains Malays.*, 1983, **12**, 249 (*synth, ir, uv-vis*)

$C_4H_6Cl_3N_2OV$ IC-003986

Bis(acetonitrile)trichlorooxovanadium(*V*), 1Cl
[33519-55-0]

$VOCl_3(NCCH_3)_2$

M 255.4
According to Brunette *et al* the bis-MeCN adduct is formed in CCl_4 soln. based on spectroscopic evidence, but only $VOCl_3.MeCN$ could be isol. Synth. from $VOCl_3$ and MeCN in CCl_4. Black solid.

Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **296**, 36 (*synth*)
Brunette, J.P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1971, **272**, 2147 (*synth in soln, uv-vis*)
Buslaev, Yu.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1978, **243**, 1175; *CA*, **90**, 114237w (*V-51 nmr*)

$C_4H_6Cl_3N_3ORu$ IC-003987

Trichlorobis(acetonitrile)(nitrosyl)ruthenium, 8Cl
Trichlorobis(methyl cyanide)(nitrosyl)ruthenium. Trichlorobis(ethanenitrile)(nitrosyl)ruthenium
[15281-56-8]

$Ru(NO)Cl_3(NCCH_3)_2$

M 319.5
Isomeric form not established; presumably similar to Trichlorobis(methyldiphenylphosphine)(nitrosyl) ruthenium, IC-011883. Red solid. Mp > 320° dec. Ir ν_{NO} 1904 cm^{-1}.

Parry, M.B. *et al*, *J. Chem. Soc. A*, 1966, 475 (*synth, ir*)

IC-003988

$C_4H_6Cl_4CrN_2^{\ominus}$

Bis(acetonitrile)tetrachlorochromate(*III*)(1 −), 10Cl

$[CrCl_4(NCCH_3)_2]^{\ominus}$

M 275.9 (ion)

cis-form
Obt. from Bis(acetic acid)tetrachlorochromate(*III*)(1 −), IC-004067 + MeCN.

Et_4N salt: [86862-39-3]
Purple solid.

Quinolinium salt: [86862-37-1]
Purple solid + MeCN. Ir ν_{max} 3322, 2292, 2247; $\nu_{C\equiv C}$ 340 cm^{-1}.

Seddon, K.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2193 (*synth, ir, uv-vis, struct*)

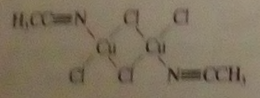
IC-003989

$C_4H_6Cl_6Cu_2N_2$

Bis(acetonitrile)di-μ-chlorodichlorodicopper(*II*), 8Cl

Tetrachlorobis(acetonitrile)dicopper. Copper(II) *chloride acetonitrile*

[17368-07-9]



M 351.0
V. hygroscopic yellow needles. Dec. at 325° to $(CuCl_2)_2(CH_3CN)_2$.

Willett, R.D. *et al*, *J. Chem. Phys.*, 1964, **40**, 838 (*synth, cryst struct*)
Willett, R.D., *J. Inorg. Nucl. Chem.*, 1967, **29**, 2482 (*ir*)
Barnes, J.C., *J. Inorg. Nucl. Chem.*, 1969, **31**, 95 (*synth, uv, ir, thermal props*)

IC-003990

$C_4H_6Cl_4HfN_2$

Bis(acetonitrile-*N*)tetrachlorohafnium(*IV*), 11Cl

Tetrachlorobis(acetonitrile)hafnium(IV)

$(MeCN)_2HfCl_4$

M 402.4
Octahedral.

cis-form [65556-77-6]
Synth. by dissolving $HfCl_4$ in dry MeCN or in soln. of MeCN in CCl_4. Also by electrochemical oxidation of Hf in the presence of Cl_2. Solid.

Brisdon, B.J. *et al*, *Spectrochim. Acta, Part A*, 1969, **25**, 999 (*synth, uv-vis, ir*)
Habeeb, J.J. *et al*, *Can. J. Chem.*, 1977, **55**, 3882 (*electrochem synth*)
Chizhikova, S.M. *et al*, *Izv. Akad. Nauk SSSR, Met.*, 1980, 86; *Russ. Metall. (Engl. Transl.)*, 1980, 80 (*nqr, thermal dec*)
Hase, Y. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 711 (*raman, ir*)
Graven, W.M. *et al*, *J. Inorg. Nucl. Chem.*, 197?, **31**, 1743 (*synth, ir*)

IC-003991

$C_4H_6Cl_4MoN_2$

Bis(acetonitrile)tetrachloromolybdenum(*IV*), 9Cl

[19187-82-7]

$MoCl_4(N{\equiv}CCH_3)_2$

M 319.8
cis-Octahedral. Synth. by treatment of $MoCl_5$ with excess MeCN. Convenient precursor for Mo(*IV*) complex formation. Air sensitive orange-brown powder (MeCN). μ_{eff} = 2.48μ_B (300K). EtCN analogue also known.

[56613-96-8, 77210-60-7]

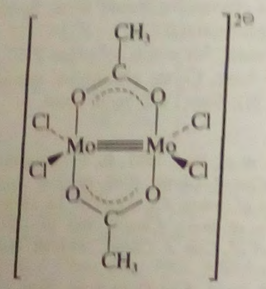
Allen, E.A. *et al*, *J. Chem. Soc.*, 1964, 4531 (*synth, ir, uv, magnetism*)
Greco, A. *et al*, *J. Organomet. Chem.*, 1973, **60**, 115 (*synth, use*)
Edwards, D.A. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1975, **5**, 139 (*synth, magnetism, ir*)
Chizhikova, S.M. *et al*, *Izv. Akad. Nauk SSSR, Met.*, 1980, 86; *CA*, **94**, 166842s (*thermal anal*)
Kan, C.T., *J. Chem. Soc., Dalton Trans.*, 1982, 2309 (*use*)
Bishop, P.T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1988, 2535 (*use*)
Pennesi, G. *et al*, *J. Chem. Res. (S)*, 1989, 86 (*use*)
Inorg. Synth., 1990, **28**, 33 (*synth, use*)

IC-003992

$C_4H_6Cl_4Mo_2O_4^{2\ominus}$

Bis[μ-(acetato-*O*:*O*′)]tetrachlorodimolybdate(*II*)(2 −), 10Cl

Di-μ-acetatotetrachlorodimolybdate(II)(2 −)



M 451.7 (ion)

Bis-Ph_4As salt: [70004-02-3].
Dark-red cryst. + $2H_2O$.

[69109-39-3]

Garner, C.D. *et al*, *Inorg. Chim. Acta*, 1978, **31**, L451 (*cryst struct*)
Clegg, W. *et al*, *Inorg. Chem.*, 1979, **18**, 2250 (*cryst struct, synth*)

IC-003993

$C_4H_6Cl_4N_2Nb$

Bis(acetonitrile)tetrachloroniobium(*IV*), 11Cl

Tetrachlorobis(methyl cyanide)niobium(IV). *Niobium*(IV) *chloride bis(acetonitrile)*

[20645-68-5]

As Bis(acetonitrile)tetrabromoniobium(*IV*), IC-003971 with

X = Cl

M 316.8

cis-form [22937-45-7]
Synth. either by heating $NbCl_4$ in MeCN under reflux or by Al reduction of $NbCl_5$ in MeCN. Pale orange-brown solid. Paramagnetic, μ_{eff} = 1.37μ_B (300K), 1.22μ_B (80K).

trans-form [100429-20-7]
Calculations on this isomer are reported by Bursten; it has not been isol.

[78407-58-6]

Fowles, G.W.A. *et al*, *Inorg. Chem.*, 1969, **8**, 631 (*synth, ir, magnetism*)
Machin, D.J. *et al*, *J. Less-Common Met.*, 1969, **19**, 405 (*synth, uv-vis, magnetism*)
Gut, R. *et al*, *J. Less-Common Met.*, 1972, **26**, 369 (*synth, from $NbCl_5$*)
Benton, J.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1304 (*cryst struct, cis-form*)
Bursten, B.E. *et al*, *Inorg. Chem.*, 1986, **25**, 831 (*electrochem, theory*)

IC-003994

$C_4H_6Cl_4N_2Re^{\ominus}$

Bis(acetonitrile)tetrachlororhenate(*III*)(1 −), 9Cl

[53290-76-9]

$[ReCl_4(NCMe)_2]^{\ominus}$

M 410.1 (ion)
cis-Octahedral at Re.

Me_3NH salt: Synth. from $ReCl_4(MeCN)_2$ in Me_2CO aq. and 40% ethanolic Me_3N in Me_2CO. Air stable orange cryst. Sol. H_2O. Paramagnetic; μ_{eff} = 1.70 μ_B (295K).
Cs salt: From $ReCl_4(MeCN)_2$ in MeCN and Cd/Hg poured into hot $CsClO_4$ in MeCN. Air-sensitive orange cryst. Readily sol. H_2O.
Cd salt (2:1): Synth. from $ReCl_4(MeCN)_2$ in MeCN and Cd/Hg. Air-sensitive orange prisms. V. sol. H_2O.

Rouschias, G. *et al*, *J. Chem. Soc. A*, 1968, 489 (*synth, ir, props*)
Rouschias, G., *Chem. Rev.*, 1974, **74**, 559, 560 (*props, struct*)
Griffith, W.P. *et al*, *J. Mol. Struct.*, 1978, **46**, 307 (*electrochem*)

IC-003995

$C_4H_6Cl_4N_2Re$

Bis(acetonitrile)tetrachlororhenium(*IV*), 9Cl

Rhenium(IV) *chloride bis(acetonitrile)*

[16853-53-5]

$ReCl_4(NCMe)_2$

M 410.1
Pseudo-octahedral. Useful intermed. for synth. of Re(*IV*) complexes.

cis-form [55332-27-9]
Synth. by (i) reduction of $ReCl_5$ by MeCN, (ii) reaction of β-$ReCl_4$ with boiling MeCN, (iii) oxidation of *fac*-$Re(CO)_3Cl(NCMe)_2$ with Cl_2. Green cryst., hydrol. by hot H_2O. Sol. polar solvs.

trans-form [55222-18-9]
Brown-green cryst.

Rouschias, G. *et al*, *J. Chem. Soc. A*, 1968, 489 (*synth, ir, magnetism, props*)
Walton, R.A. *et al*, *Inorg. Chem.*, 1971, **11**, 2534 (*synth, props*)
Edwards, D.A. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1974, **4**, 573 (*synth, struct, props*)
Myers, R.E. *et al*, *Inorg. Chem.*, 1976, **15**, 3065 (*synth, props*)

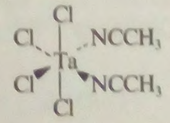
IC-003996

$C_4H_6Cl_4N_2Ta$

Bis(acetonitrile)tetrachlorotantalum(*IV*), 11Cl

Tantalum(IV) *chloride bis(acetonitrile)*

[22937-47-9]



M 404.8
cis-octahedral. Synth. from $TaCl_4$ and excess MeCN, or by electrochem. reduction of $TaCl_5$.MeCN. Brown solid. Paramagnetic, μ_{eff} = 0.45μ_B (293K).

Fowles, G.W.A. *et al*, *Inorg. Chem.*, 1969, **8**, 631 (*synth, ir, uv-vis, magnetism*)
Bursten, B.E. *et al*, *Inorg. Chem.*, 1986, **25**, 831 (*synth, electrochem*)

IC-003997

$C_4H_6Cl_4N_2Ti$

Bis(acetonitrile)tetrachlorotitanium(*IV*), 11Cl

Titanium(IV) *chloride bis(acetonitrile)*

[16920-98-2]

$(H_3CCN)_2TiCl_4$

M 271.7
Octahedral.

cis-form [16969-37-2]
Synth. by dissolving $TiCl_4$ in MeCN or by electrochemical oxidation of Ti in MeCN in the presence of Cl_2. Yellow solid. Sol. MeCN.

Brisdon, B.J. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 1969 (*uv-vis*)
Perkins, P.G. *et al*, *J. Chem. Soc. A*, 1970, 3229 (*thermochem*)
Kawano, Y. *et al*, *J. Mol. Struct.*, 1976, **30**, 45 (*ir, raman*)
Habeeb, S.J. *et al*, *Can. J. Chem.*, 1977, **55**, 3882 (*electrochem synth, ir*)
Troyanov, S.I. *et al*, *Koord. Khim.*, 1985, **11**, 1147; *CA*, **103**, 151297y (*synth, cryst struct*)

IC-003998

$C_4H_6Cl_4N_2V$

Bis(acetonitrile)tetrachlorovanadium(*IV*), 8Cl

Tetrachlorobis(methyl cyanide)vanadium(IV). *Varadium*(IV) *chloride bis-acetonitrile*

[31204-53-2]

$VCl_4(NCCH_3)_2$

M 274.8
Octahedral: detailed geometry is unknown. Synth. by adding VCl_4 to MeCN in CCl_4. Purple-black solid. Readily hydrol. With excess MeCN reduction to VCl_3.3MeCN occurs. Sol. C_6H_6. Subl. 80° *in vacuo*. Paramagnetic, μ_{eff} = 1.77μ_B (293K).

Duckworth, M.W. *et al*, *J. Chem. Soc.*, 1963, 5665 (*synth, uv-vis*)

IC-003999

$C_4H_6Cl_4N_2W$

Bis(acetonitrile)tetrachlorotungsten(*IV*), 11Cl, 9Cl, 8Cl

Tetrachlorobis(acetonitrile)tungsten. Tungsten(IV) *chloride bis(acetonitrile)*

[12073-20-0]

$WCl_4(NCCH_3)_2$

M 407.7
Octahedral. Starting material.

cis-form
Synth from WCl_5 + $W(CO)_6$ in MeCN. Red solid.

[40354-88-9]

Allen, E.A. *et al*, *J. Chem. Soc.*, 1964, 4531 (*synth, props*)
King, M.A.S. *et al*, *Inorg. Chem.*, 1973, **12**, 1972 (*synth, ir*)
Edwards, D.A. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1975, **5**, 139 (*synth*)

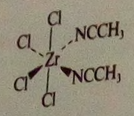
IC-004000

$C_4H_6Cl_4N_2Zr$

Bis(acetonitrile)tetrachlorozirconium(*IV*), 11Cl

Zirconium(IV) *chloride bis-acetonitrile*

[12073-21-1]



M 315.1

cis-form [65556-76-5]

Synth. from $ZrCl_4$ + MeCN. Colourless solid, dec. in MeOH. Insol. CCl_4, hexane. Mp 194-197° dec.

Fowles, G.W.A. *et al*, *J. Chem. Soc.*, 1964, 2840 (*synth, uv-vis*)
Feltz, A., *Z. Anorg. Allg. Chem.*, 1965, **335**, 304 (*reactions*)
Graven, W.M. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 1743 (*synth, ir*)
Troyanov, S.I. *et al*, *Koord. Khim.*, 1986, **12**, 1000; *CA*, **105**, 106175n (*cryst struct, cis-form*)

IC-004001

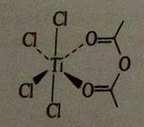
$C_4H_6Cl_4O_3Ti$

(Acetic anhydride)tetrachlorotitanium(*IV*)

(*Acetic acid anhydride*)*tetrachlorotitanium*(IV), *11Cl*.

Titanium(IV)*chloride acetic anhydride*

[12073-24-4]



M 291.7

Octahedral. Synth. by reaction of $TiCl_4$ with Ac_2O in acetyl chloride soln. or by reaction of $TiOCl_2$ or $Ti(OAc)Cl_3$ with acetyl chloride. Yellow solid. Dec. to (Acetato-*O*)trichlorotitanium(*IV*), IC-003063 on heating.

Viard, B. *et al*, *J. Chem. Res.* (*S*), 1983, 84 (*synth, cryst struct, ir*)

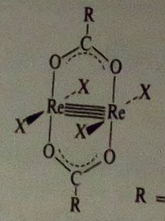
IC-004002

$C_4H_6Cl_4O_4Re_2$

Bis[μ-(acetato-*O,O'*)]tetrachlorodirhenium(*III*), 10Cl

Rhenium(III) *acetate dichloride dimer*

[62320-69-8]



R = CH_3, X = Cl

M 632.3

Interatomic distance: Re—Re 211.1 pm. Possesses D_{2h} symmetry. Orange solid. Several solvates known.

Dihydrate: Synth. from K_2ReCl_6 or $KReO_4$, HCl, HOAc and H_2 in autoclave. Dark blue cryst.

[29131-21-3]

Cotton, F.A. *et al*, *Inorg. Chem.*, 1965, **4**, 326; 1967, **6**, 223 (*synth*)
Koz'min, P.A. *et al*, *Zh. Strukt. Khim.*, 1970, **11**, 313; *J. Struct. Chem. USSR* (*Engl. Transl.*), **11**, 291.
Koz'min, P.A. *et al*, *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1979, **5**, 1201.
Shtemenko, A.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1980, **25**, 704 (*synth, uv*)
Cotton, F.A. *et al*, *Multiple Bonds Between Metal Atoms*, Wiley, New York, 1982, 38 (*bibl, struct*)

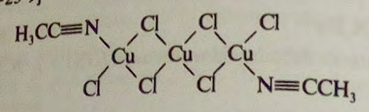
IC-004003

$C_4H_6Cl_6Cu_3N_2$

Bis(acetonitrile)tetra-μ-chlorodichlorotricopper(*II*), 8Cl

Hexachlorobis(*acetonitrile*)*tricopper*(II)

[17732-23-9]



M 485.4

Hygroscopic, short, dark-red needles. Dec. at 325° to $(CuCl_2)_5(CH_3CN)_2$.

Willett, R.D. *et al*, *J. Chem. Phys.*, 1964, **40**, 838 (*synth, cryst struct*)
Willett, R.D., *J. Inorg. Nucl. Chem.*, 1967, **29**, 2482 (*uv*)
Barnes, J.C., *J. Inorg. Nucl. Chem.*, 1969, **31**, 95 (*synth, thermal props, ir, uv*)

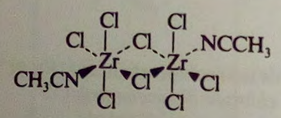
IC-004004

$C_4H_6Cl_8N_2Zr_2$

Bis(acetonitrile)di-μ-chlorohexachlorodizirconium(*IV*), 11Cl

Di-μ-chlorobis[(*acetonitrile*)*trichlorozirconium*(IV)]

[106452-83-9]



M 548.1

Troyanov, S.I. *et al*, *Koord. Khim.*, 1986, **12**, 1276; *CA*, **106**, 59227 (*cryst struct*)

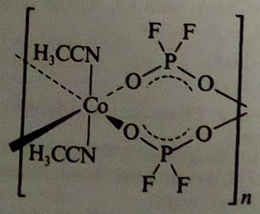
IC-004005

$C_4H_6CoF_4N_2O_4P_2$

Bis(acetonitrile)bis(difluorophosphato)cobalt(*II*)

Bis(*acetonitrile*)*bis*(*phosphorodifluoridato-*O)*cobalt*(II), *11Cl*

[100811-52-7]



M 342.9

Polymeric chain struct. with octahedral Co. V. hygroscopic red cryst.

Begley, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 2433 (*synth, ir, cryst struct*)

IC-004006

$C_4H_6CoO_4$

Cobalt(*II*) acetate($Co(OAc)_2$)

[71-48-7]

$Co(OAc)_2$

M 177.0

Prepared commercially from $Co(OH)_2$ or CoO_3 + excess dil. AcOH. Oxidation catalyst. Light pink cryst. V. sol. H_2O; sol. EtOH.

▷ Toxic. AG3150000.

Tetrahydrate: see *Bis*(*acetato-*O)*tetraaquacobalt*, *IC-004299*

Fernandez, G.J. *et al*, *Rev. Acad. Cienc. Exactas, Fis., Quim. Nat. Zaragoza*; *CA*, **81**, 55385g (*cryst struct*)
Paul, R.C. *et al*, *Indian J. Chem.*, 1972, **10**, 939 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 99 (*use*)
Boraldi, P. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 89 (*ir*)
Marshall, G.L., *Org. Mass Spectrom.*, 1983, **18**, 168 (*ms*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 940.

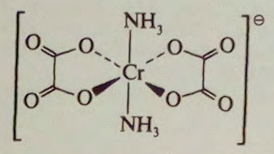
IC-004007

$C_4H_6CrN_2O_8^{\ominus}$

Diamminebis(oxalato)chromate(*III*)(1 –)

Diamminebis[*ethanedioato*(2 –)-O,O']*chromate*(1 –), *9Cl*

[54053-39-3]



M 262.0 (ion)

Believed to be *trans*-octahedral from esr measurements.

K salt: No phys. props. reported.

Tetraammineoxalatochromium(III)(*1+*) *salt:* [20631-59-8].
$C_6H_{18}Cr_2N_6O_{12}$ M 470.2
Violet powder.

Kyuno, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 1848 (*synth, uv*)
Garner, C.S. *et al*, *Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Andriessen, W.T.M., *Inorg. Chem.*, 1975, **14**, 792 (*esr*)

IC-004008

$C_4H_6CrN_6S_4^{\ominus}$

Diamminetetrakis(thiocyanato-*N*)chromate(*III*)(1 –), 11Cl, 10Cl, 9Cl

Diamminetetrathiocyanatochromate(III)

[16248-93-4]

$[Cr(NCS)_4(NH_3)_2]^{\ominus}$

M 318.3 (ion)

trans-Octahedral. Used as a starting material. Forms spar. sol. salts with cations. V. many salts and derivs. known.

K salt: [34430-73-4].
Synth. aq. NH_4 salt + KNO_3. Light-sensitive solid (aq. KNO_3).

NH_4 salt, monohydrate: [13573-16-5]. *Reinecke's salt*
Synth. from NH_4SCN fused with $(NH_4)_2Cr_2O_7$ and product extracted with H_2O. Light-sensitive ruby-red cryst. (H_2O). Sol. H_2O, EtOH, Me_2CO; insol. C_6H_6, dec. by boiling H_2O. Treatment with aq. HCl and extraction with Et_2O gives $H[Cr(NCS)_4(NH_3)_2]$.

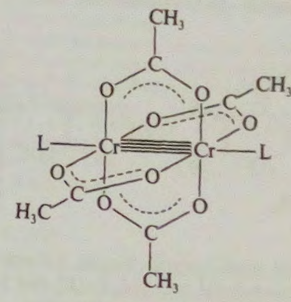
Takeuchi, Y. *et al*, *Z. Kristallogr.*, 1957, **109**, 29 (*cryst struct*)
Bennett, M.A. *et al*, *Inorg. Chem.*, 1967, **6**, 1625 (*synth, uv, ir*)
Garner, C.S. *et al*, *Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1516 (*synth*)
Rojas, G.E. *et al*, *J. Phys. Chem.*, 1986, **90**, 87 (*flash photol*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 837 (*rev*)

IC-004009

$C_4H_6CrO_4$

Chromium(*II*) acetate

Chromous acetate



dimer, L = donor ligand or O from adjacent molecule

M 170.0

Dimeric, many carboxylato analogues: e.g. R = H, *tert*-Bu, CF_3, Ph, and derivs. known. Strong reducing agent; starting material.

Tetrakis*[*μ-(acetato-O:O')*]*dichromium*(*II*), *11Cl, 10Cl, 9Cl

[15020-15-2]

Dimer
$C_8H_{12}Cr_2O_8$ M 340.1
Cr—Cr 228.8 pm. Obt. by thermal dehydration of hydrate. Prototype for many quadruply bonded Cr_2 compds. Yellow-brown cryst. (by subl.).

▷ Pyrophoric.

Dihydrate: [628-52-4]. *Tetrakis*[*μ-*(*acetato-*O:O')]*diaquadichromium*, *11Cl, 10Cl, 9Cl*
Reducing agent, starting material. Air-sensitive dark red cryst. (H_2O). Stable in air for short period. Spar. sol. H_2O, EtOH; sol. hot H_2O. Loses H_2O at 100°. Cr—Cr, 236.2 Cr—OH_2, 227.2 pm.

▷ AG3000000.

Di-NH_3 complex: [75576-28-2]. *Tetrakis*[*μ-*(*acetato-*O:O')]*diamminedichromium*, *10Cl*
$C_8H_{18}Cr_2N_2O_8$ M 374.2
Reddish purple, air-sensitive solid. $\mu_{eff} = 0.6\mu_B$ (295K), $0.3\ \mu_B$ (90K).

Bis-acetic acid complex: [15225-50-0]. *Tetrakis*[*μ-*(*acetato-*O:O')]*bis*(*acetic acid*)*dichromium*
Red needles (AcOH). Cr—Cr 230.0 pm.

Bis-Py complex: [66197-70-4]. *Tetrakis*[*μ-*(*acetato-*O:O')]*bispyridinedichromium*
$C_{18}H_{22}Cr_2N_2O_8$ M 498.3
Red prisms (aq. Py). Cr—Cr 236.9, Cr—N 233.5 pm.

Bis-piperidine complex:
$C_{18}H_{34}Cr_2N_2O_8$ M 510.4
Red-purple leaflets (piperidine). Cr—Cr 234.2 pm.

Bis(*4-cyanopyridine*) *complex:* Red cryst. (THF/hexane). Cr—Cr 231.5, Cr—N 232.7 pm.

Pyrazine complex: [72186-99-3]. *Tetrakis*[*μ-*(*acetato-*O:O')]*pyrazinedichromium*
Reddish orange cryst. Pyrazine links $Cr_2(OAc)_4$ units in chains. Cr—Cr 229.5, Cr—N 231 pm.

[14404-41-2, 29826-26-4, 92141-39-4]

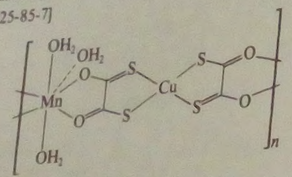
Inorg. Synth., 1966, **8**, 125 (*synth*)
Cotton, F.A. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 1684 (*cryst struct*)
Fieser and Fieser, Reagents for Organic Synthesis, 1977, **6**, 4, 5, 487 (*uses*)
Cotton, F.A. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 4704 (*cryst struct*)
Cotton, F.A. *et al*, *Nouv. J. Chim.*, 1984, **8**, 331 (*derivs*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 717, 740 (*rev, uses*)

$C_4H_6CuMnO_7S_4$ IC-004010

Triaquabis(μ-dithiooxalato)copper(*II*)manganese(*II*)

Triaqua[(copper)(μ-ethanebis(thioato)(2−)-O,O′:S,S′]][ethanebis(thioato)(2−)-O,O′]manganese, 11Cl

[90025-85-7]



M 412.8

Polymeric struct. with 7-coord. Mn(*II*). Ferromagnetic quasi-one-dimensional material. Cu(*II*) and Mn(*II*) are antiferromagnetically coupled at low temp.

4.5 Hydrate: [89958-80-5].

Synth. from a warm aq. slurry of $K_2Cu(S_2C_2O_2)_2$ with conc. aq. $MnSO_4$. Brown ribbon shaped cryst. (H_2O).

Gleizes, A. *et al, J. Am. Chem. Soc.*, 1984, **106**, 3727 (*synth, cryst struct, magnetism*)

$C_4H_6CuN_4O_6$ IC-004011

Bis(acetonitrile)dinitratocopper(*II*)

Copper(II) *nitrate acetonitrile complex (1:2)*

[14518-16-2]

$Cu(NO_3)_2(NCCH_3)_2$

M 269.6

Each Cu has tetragonal pyramidal coordination with half the nitrate groups bridging, forming infinite chains. MeCN molecules *trans*. Deep blue cryst. (MeCN).

Duffin, B., *Acta Crystallogr., Sect. B*, 1968, **24**, 396 (*synth, cryst struct*)

$C_4H_6F_2O_{10}S_2Zr$ IC-004012

Bis(acetato-*O,O′*)bis(fluorosulfato-*O,O′*)zirconium(*IV*), 11Cl

[81789-59-5]

$Zr(OAc)_2[OS(O)_2F]_2$

M 407.4

The bidentate nature of the ligands is based on ir evidence. Synth. by adding fluorosulfuric acid to $Zr(OAc)_4$ in sulfuryl chloride. White solid. Forms adducts with Py and bipy.

Sing, S. *et al, J. Fluorine Chem.*, 1982, **20**, 107 (*synth, ir, thermal anal*)

$C_4H_6FeGe_2O_4$ IC-004013

Tetracarbonyldigermyliron, 8Cl

As Tetracarbonylbis(trichlorogermyl)iron, IC-003852 with

X = H

M 319.1

cis-form [33248-48-5]

Colourless volatile solid. Mp 71°.

Stobart, S.R., *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 219 (*synth, ir, pmr*)

$C_4H_6FeO_4$ IC-004014

Iron(*II*) acetate

Ferrous acetate. Iron(II) *ethanoate. Ferrous ethanoate. Acetic acid, iron(2+) salt*

[3094-87-9]

$Fe(OAc)_2$

M 173.9

Synth. from $Fe(CO)_5$ + HOAc and Ac_2O in DMF. White or colourless cryst. $\mu_{eff} = 5.19\mu_B$.

▷ AI3850000.

Tetrahydrate: Used for textile dyeing; wood preservative. Green cryst., oxidises in air. Sol. H_2O, EtOH. Dec. on heating.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1930, **B**, 521 (*rev, bibl*)

Hardt, H.D. *et al, Z. Anorg. Allg. Chem.*, 1961, **313**, 57 (*synth*)

Calderazzo, F. *et al, J. Chem. Soc. A*, 1969, 1378 (*synth, ir*)

Fernandez, G.J. *et al, Rev. Acad. Cienc. Exactas, Fis., Quim. Nat. Zaragoza*, 1973, **28**, 303 (*struct*)

Catterick, J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1420 (*ir, uv, synth*)

$C_4H_6FeO_4Si_2$ IC-004015

Tetracarbonyldisilyliron, 10Cl, 8Cl

[26469-80-7]

As Tetracarbonylbis(trichlorosilyl)iron, IC-003853 with

X = H

M 230.1

cis-form [14465-62-4]

White solid, readily sublimed at r.t. Mp 52°. Turns pale-yellow at 85°, dec. above 110°.

▷ Explodes violently in air.

Bancroft, G.M. *et al, Discuss. Faraday Soc.*, 1969, 136 (*mössbauer*)

Aylett, B.J. *et al, J. Chem. Soc. A*, 1969, **14**, 2110 (*synth, ir, pmr*)

Aylett, B.J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2058.

$C_4H_6HgO_4$ IC-004016

Mercury acetate

*Bis(acetato-*O*)mercury*(II). *Mercuric acetate*

[1600-27-7]

$Hg(OAc)_2$

M 318.6

Covalently bonded in aq. soln. Oxidation catalyst; mercurating agent; used in photosensitive materials, in photothermographic copying compositions; trans-etherification and esterification catalyst. White cryst., photosensitive. Sol. H_2O, AcOH. Mp 178-180°. Undergoes free radical dec. on photolysis or in presence of peroxides. Rapid dec. at 280°.

▷ AI8575000.

Mahaptra, P. *et al, J. Indian Chem. Soc.*, 1953, **30**, 509 (*stability const*)

Bernard, M.A. *et al, Bull. Soc. Chim. Fr.*, 1967, 4649 (*thermal anal*)

Cooney, R.P.J. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 1519 (*ir, raman in solid state and soln*)

Allman, R., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1973, **138**, 366 (*cryst struct*)

Borzo, M. *et al, J. Magn. Reson.*, 1975, **19**, 279 (*Hg-199 nmr*)

Barron, P.F., *J. Organomet. Chem.*, 1982, **236**, 157 (*solid state cmr*)

Jagannathan, N.R. *et al, Indian J. Pure Appl. Phys.*, 1984, **22**, 484 (*pmr*)

Gerbeleu, N.V. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1984, **29**, 169 (*ms*)

Harris, R.K. *et al, Magn. Reson. Chem.*, 1987, **25**, 1058 (*solid state nmr*)

Tackett, J.E., *Appl. Spectrosc.*, 1989, **43**, 483 (*soln ir*)

Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2190.

$C_4H_6Hg_2O_4$ IC-004017

Mercury(*I*) acetate

*Bis(acetato-*O*)dimercury. Mercurous acetate*

[631-60-7]

AcOHgHgOAc

M 519.2

Synth. from $Hg_2(NO_3)_2.2H_2O$ and NaOAc in dil. HNO_3. Bactericide. Light-sensitive colourless needles (aq. AcOH). Sol. H_2O (0.75 g per 100 cm^3 at 15°, dec.), sol. dil. HOAc; insol. EtOH, Et_2O. Disproportionates to Hg and $Hg(OAc)_2$ on boiling aq. soln. or in light. Dec. at 250°.

▷ AI8570000.

Gowenlock, B.G. *et al, J. Chem. Soc.*, 1955, 1454 (*uv*)

Ludwig, G.W., *J. Chem. Phys.*, 1956, **25**, 159 (*pmr*)

Puff, H. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1965, **122**, 156.

Dorm, E. *et al, Acta Chem. Scand.*, 1967, **21**, 1661 (*powder struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 34, 1968, **B3**, 1266 (*rev, bibl*)

Cooney, R.P.J. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 1519 (*raman, ir*)

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1063 (*synth*)

Balyatinskaya, L.N., *Zh. Fiz. Khim.*, 1978, **52**, 1347.

Nefedov, V.I. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1425 (*pe*)

Volkov, V.E. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 205 (*raman*)

Merck Index, 11th Ed., 1989, No. 5792.

$C_4H_6MgO_4$ IC-004018

Magnesium acetate

Acetic acid, magnesium salt, 8Cl. Ethanoic acid, magnesium salt

[142-72-3]

$Mg(OAc)_2$

M 142.3

Synth. by heating the tetrahydrate to ~100° *in vacuo*. Catalyst for the polym. of alkenes. White powder. V. sol. H_2O; sol. MeOH. Mp 357°. ΔH_f° −1367.7 kJ mol^{-1}. High temp. calcination leads to MgO.

▷ AI5600000.

Tetrahydrate: [16674-78-5].

$C_4H_{14}MgO_8$ M 214.4

Cryst. from aq. soln. of $Mg(OAc)_2$ obt. by neutralisation of aq. $Mg(OH)_2$ by aq. AcOH. Commercially available. Deliquescent colourless monoclinic cryst. Dec. on heating to form amorphous $Mg(OAc)_2$ at ~160°, crystalline $Mg(OAc)_2$ at ~200° and MgO at ~300°. V. sol. H_2O (120 g per 100 cm^3 at 15°), EtOH. Mp 80°. ΔH_f° −2566.1 kJ mol^{-1}. Dehyd. by $(MeO)_2CMe_2$ in MeOH gives $Mg(OAc)_2.2MeOH.2H_2O$.

Padmanabhan, V.M., *Proc. Indian. Acad. Sci., Sect. A*, 1953, **37**, 401; *CA*, **47**, 8515a (*raman, tetrahydrate*)

Shankar, J. *et al, Proc. Indian. Acad. Sci., Sect. A*, 1957, **45**, 117; *CA*, **51**, 11805 (*cryst struct, tetrahydrate*)

Vranty, F. *et al, Anal. Chem.*, 1961, **33**, 1455 (*ir*)

Manabe, K. *et al, Kogyo Kagaku Zasshi*, 1967, **70**, 13; *CA*, **67**, 78612 (*thermal dec, tetrahydrate*)

Padmanabhan, A.C. *et al, Indian J. Pure Appl. Chem.*, 1973, **11**, 404 (*pmr, tetrahydrate*)

Murata, S. *et al, Netsu Sokutei*, 1977, **4**, 89; *CA*, 1978, **89**, 169988 (*thermochem data, anhyd, tetrahydrate*)

Herrera, J. *et al, Circ. Farm.*, 1981, **39**, 153; *CA*, 1982, **96**, 27722 (*dehydration, tetrahydrate*)

Baraldi, P. *et al, Spectrochim. Acta, Part A*, 1981, **37**, 89; 1982, **38**, 51 (*synth, ir, anhyd, thermal dec, ir, tetrahydrate*)

Jagannathan, N.R. *et al, Indian J. Pure Appl. Phys.*, 1984, **22**, 484; *CA*, **101**, 203010 (*pmr*)

Gardner, T.J. *et al, Thermochim. Acta*, 1984, **78**, 17 (*thermal dec, anhyd, tetrahydrate*)

Raghuvanshi, G.S. *et al, J. Solid State Chem.*, 1985, **57**, 207 (*ir, raman, tetrahydrate*)

$C_4H_6MnN_2OS$ IC-004019

Dicyano(dimethyl sulfoxide)manganese(*II*)

*Bis(cyano-*C*)[sulfinylbis(methane)-*O*]manganese, 10Cl*

[71072-47-4]

$Mn(Cn)_2O{=}SMe_2$

M 185.1

Polymeric struct. with octahedral Mn and bridging CN. Synth. by passing $[NH_4]CN$ in an N_2 stream through anhydrous $MnBr_2$ in DMSO. Light brown solid, air-stable.

Kuntyi, O.I. *et al, Sov. J. Coord. Chem.* (*Engl. Transl.*), 1979, **5**, 539 (*synth, ir, powder struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 98 (*rev, bibl*)

$C_4H_6MnN_2S_4$ IC-004020

[Ethylenebis(dithiocarbamato)]manganese, 8Cl

[1,2-Ethanediylbis[carbamodithioato](2−)]manganese(II), *9Cl. Maneb, BSI, ISO. Dithiane M-22. Manzate. Farmaneb. MEB. Numerous proprietary names*

[12427-38-2]

$[MnS_2CNHCH_2CH_2NHCS_2]_n$

M 265.3

Polymeric chain struct., geometry about Mn not known. Synth. from Mn(*II*) salts and Na salt of ligand. Fungicide esp. for protection of potatoes and tomatoes. Yellow cryst., slow dec. on prolonged exp. to air, rapid dec. in acid. May be stabilised by presence of formaldehyde or various other compds. Insol. H_2O, common org. solvs. Mp 131° dec. Forms a dihydrate, adducts with NH_3 and dodecylamine.

▷ OP0700000.

Kozlov, G.A. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 396 (*synth, ir, dihydrate*)

Kwoka, W. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 1889 (*synth, magnetism, ir*)

Schmandke, H. *et al, CA*, 1985, **103**, 18079 (*tox*)

Gergely, S. *et al, Chem. Zvesti*, 1988, **42**, 229 (*struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 180 (*rev, bibl*)

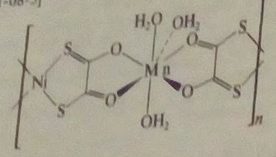
Pesticide Manual, 9th Ed., 1991, No. 7770.

$C_4H_6MnNiO_7S_4$ IC-004021

Triaquabis(dithiooxalato)nickelmanganese

Triaqua[μ-[ethanebis(thioato)(2−)-O,O′:S,S′]][[ethanebis(thioato)(2−)-S,S′]nickel]manganese, 10CI

[79791-08-5]



M 407.9

Stacked chain struct. separated by intervening H_2O molecules. Pentagonal bipyramidal Mn(*II*). Synth. from conc. aq. solns. of $K_2Ni(S_2C_2O_2)_2$ and $MnSO_4$. Air-stable black ribbon shaped cryst. + $4.5H_2O$ (H_2O). Paramagnetic.

[89958-81-6]

Gleizes, A. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 7373; 1984, **106**, 3727.

$C_4H_6MnO_4$ IC-004022

Manganese(*II*) acetate

Manganese diacetate. Manganese diethanoate

[638-38-0]

$Mn(OAc)_2$

M 173.0

Forms mono-, di-, and tetrahydrates but little is known about the mono-, and dihydrates. Synth. by heating the tetrahydrate with acetic anhydride. Forms complex anions $[Mn(OAc)_4]^{2\ominus}$. Sol. H_2O, MeOH, EtOH, AcOH; insol. Me_2CO. Mp *ca.* 210°. Tetragonal struct. μ_{eff} = $5.56\mu_B$ (292 K).

▷ AI5770000.

Tetrahydrate: [15243-27-3].

Synth. from $MnCO_3$ and AcOH. Red cryst. Struct. contains MnO_6 and *cis*- $MnO_4(H_2O)_2$ octahedra. Exhibits complex magnetic behaviour.

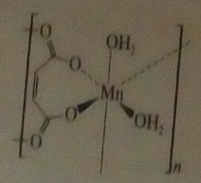
Edwards, D.A. *et al*, *Can. J. Chem.*, 1968, **46**, 3443 (*synth*)
Mehr, A. *et al*, *J. Chem. Phys.*, 1968, **48**, 4381 (*uv*)
Buriet, P. *et al*, *Solid State Commun.*, 1974, **14**, 665 (*magnetism*)
Tranqui, D. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1357 (*cryst struct*)
Wood, T.E. *et al*, *Inorg. Chem.*, 1979, **18**, 2936 (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 29 (*rev, bibl*)

$C_4H_6MnO_6$ IC-004023

Diaqua[2-butenedioato(2−)-*O,O′*]manganese(*II*), 11CI

Diaqua(μ3-maleato)manganese(II)

[84825-95-6]



M 205.0

Polymeric struct. with bridging maleates and octahedral Mn (each maleate coord. to 3Mn). Synth. by boiling maleic acid and excess aq. $MnCO_3$ until the pH increases to *ca.* 7. Nearly colourless plates + $1H_2O$.

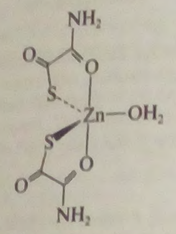
Lis, T., *Acta Crystallogr., Sect. C*, 1983, **39**, 39 (*synth, cryst struct*)

$C_4H_6N_2O_5S_2Zn$ IC-004024

Bis(aminooxoethanethioato-*O*³,*S*⁴)aquazinc, 11CI

Aquabis(1-thiooxamato)zinc

[98628-66-1]



M 291.6

Trigonal bipyramidal. Cryst. $+1H_2O$ (H_2O).

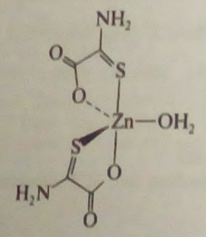
Bertels, J. *et al*, *Z. Naturforsch., B*, 1985, **40**, 1068 (*synth, cryst struct*)

$C_4H_6N_2O_5S_2Zn$ IC-004025

Bis(aminothioacetato-*O,S*)aquazinc, 11CI

Aquabis(2-thiooxamato)zinc

[98644-80-5]



M 291.6

Cryst.

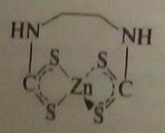
Bertels, J. *et al*, *Z. Naturforsch., B*, 1985, **40**, 1068 (*synth, cryst struct*)

$C_4H_6N_2S_4Zn$ IC-004026

[Ethylenebis(dithiocarbamato)]zinc, 8CI

[[1,2-Ethanediylbis[carbamodithioato]](2−)]zinc, 9CI. Zineb, BSI

[12122-67-7]



M 275.7

Fungicide. Moisture- and light-unstable pale yellow powder, or cryst. ($CHCl_3$/EtOH). Sol. CS_2, Py; v. sl. sol. H_2O. Dec. at 157°.

▷ Irritant. Affects alcohol + aldehyde dehydrogenases in the liver. Incompatible with Cu, Hg salts. ZH3325000.

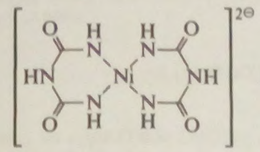
Halls, D.J. *et al*, *Anal. Chim. Acta*, 1968, **41**, 63 (*synth, polarog*)
Nicholas, M.L. *et al*, *J. Assoc. Off. Anal. Chem.*, 1976, **59**, 1266 (*raman*)

Dolmanova, I.F. *et al*, *J. Anal. Chem. USSR* (*Engl. Transl.*), 1977, **32**, 638 (*anal*)
Hylin, J.W. *et al*, *Bull. Environ. Contam. Toxicol.*, 1978, **20**, 840; *CA*, **90**, 181388j (*uv*)
Gustafsson, K.H. *et al*, *J. Agric. Food Chem.*, 1981, **29**, 729 (*hplc*)
Gheorghe, S.M. *et al*, *CA*, 1983, **99**, 121853 (*manuf*)
Srivastava, S.P. *et al*, *J. Liq. Chromatogr.*, 1983, **6**, 139 (*tlc*)
Lisi, P. *et al*, *Contact Dermatitis*, 1986, **15**, 266; 1987, **17**, 212; *CA*, **106**, 114892e; **108**, 17485h (*tox*)
Zagidullin, R.N., *Zh. Prikl. Khim.* (*Leningrad*), 1987, **60**, 1829 (*synth*)
Gergely, S. *et al*, *Chem. Zvesti*, 1988, **42**, 299 (*synth, cryst struct*)
European Directory of Agrochemical Products, 3rd Ed., Royal Society of Chemistry, 1988, **1**, 726 (*rev, use*)
Nehez, M. *et al*, *Regul. Toxicol. Pharmacol.*, 1988, **8**, 37; *CA*, **108**, 191980a (*haz*)
Pesticide Manual, 9th Ed., 1991, 866 (*rev*)

$C_4H_6N_6NiO_4^{2\ominus}$ IC-004027

Bis(biureto)nickelate(*II*)(2−)

Bis[imidodicarbonimidic diamidato(2−)-N,N′]nickelate(II) (2−), 9CI



M 260.8 (ion)

Deprotonated biuret probably coordinates through N atoms as shown.

Di-K salt, dihydrate: [15380-07-1].
$C_4H_{10}K_2N_6NiO_6$ M 375.0
Yellow powder.

McLellan, A.W. *et al*, *J. Chem. Soc. A*, 1967, 137 (*synth, ir, uv, magnetism*)
Kedzia, B.B. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 849 (*synth, ir*)

$C_4H_6N_6NiS_4^{2\ominus}$ IC-004028

Diamminetetrakis(thiocyanato-*N*)nickelate(*II*)(2−)

$[Ni(NCS)_4(NH_3)_2]^{2\ominus}$

M 325.0 (ion)

trans-Octahedral anion.

Di-NH_4 salt: Deliquescent dark-blue cubic cryst. $+H_2O$. V. sol. H_2O, sol. EtOH. μ = $3.17\mu_B$.

Porai-Koshits, M.A., *Acta Crystallogr.*, 1957, **10**, 784.
Porai-Koshits, M.A., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1959, **4**, 332 (*cryst struct*)
Yukhno, E.R., *Zh. Neorg. Khim.*, 1962, **7**, 807; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, **7**, 417 (*synth, magnetism*)

$C_4H_6NiO_4$ IC-004029

Nickel(*II*) acetate

Bis(acetato)nickel, 8CI

[373-02-4]

$Ni(OAc)_2$

M 176.7

Octahedral coord. Ni, acetates bidentate, isomorphous with anhyd. acetates of Co, Fe(*II*). Hygroscopic green powder. Dec. on heating. μ_{eff} = $3.21\mu_B$.

▷ Poison. Experimental neoplastigen and tumorigen. QR6125000.

Tetrahydrate: [6018-89-9]. *Bis(acetato-O)tetraaquanickel*(II)
$C_4H_{14}NiO_8$ M 248.8

Commercially available starting material for Ni(*II*) complexes. Green cryst. Sol. H_2O, alcohols. Isomorphous with Co analogue. μ_{eff} = $3.30\mu_B$. All four H_2O bond to nickel in *trans*-octahedral molecules.

▷ QR6126000.

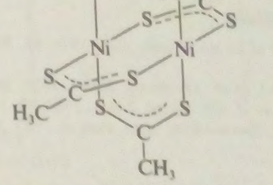
[14998-37-9, 21263-98-9]

Davis, T.L. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 1276 (*synth*)
Leicester, J. *et al*, *J. Appl. Chem.*, 1962, **12**, 357.
van Niekerk, J.N. *et al*, *Acta Crystallogr.*, 1963, **6**, 609 (*hydrate, cryst struct*)
Doremieux, J.-L., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1965, **261**, 4426.
Mookherjee, A. *et al*, *Physica* (*Amsterdam*), 1965, **31**, 1540 (*magnetism*)
Gmelin Handbook Inorg. Chem., Syst No. 57, 1966, **B3**, 860 (*rev*)
Hardt, H.D. *et al*, *Z. Anorg. Allg. Chem.*, 1966, **343**, 92 (*anhyd salt*)
Downie, T.C. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 706 (*cryst struct*)
Wendlandt, W.W. *et al*, *Thermochim. Acta*, 1974, **9**, 101 (*dta*)
Cramer, R.E. *et al*, *Inorg. Chem.*, 1975, **14**, 2462 (*hydrate, cryst struct*)
Bavadi, P. *et al*, *Spectrochim. Acta*, 1981, **37**, 89; 1982, **38**, 51 (*ir*)
Raghuvanshi, G.S. *et al*, *J. Solid State Chem.*, 1985, **57**, 207 (*ir, raman*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2478 (*tox*)

$C_4H_6NiS_4$ IC-004030

Nickel(*II*) dithioacetate

Bis(dithioacetato)nickel, 8CI



dimer

M 241.0

Dimeric.

Dimer: [95974-45-1]. *Tetrakis[μ-[ethane(dithioato)-S:S′]]dinickel, 11CI*
$C_8H_{12}Ni_2S_8$ M 482.0
Red-black cryst. (CS_2). Sol. CS_2, Py, $CHCl_3$. Mp 134-136°. Ni has effective 5-coord. coordn. (Ni-Ni 256 pm). Distant sulfurs (at 292 pm) in neighbouring molecules.

Furlani, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2404 (*synth, uv-vis*)
Bellitto, C. *et al*, *Inorg. Chem.*, 1985, **24**, 2815 (*synth, ir, uv-vis, cryst struct, pe*)

$C_4H_6O_2RuS_2$ IC-004031

Dicarbonylbis(methanethiolato)ruthenium(*II*), 9CI

[32005-89-3]

$[Ru(CO)_2(SMe)_2]_n$

M 251.2

Polymeric or oligomeric compd., structs. ranging from chains to clusters have been postulated. Prepd. by treating $Ru_3(CO)_{12}$ with MeSH or S_2Me_2. Ir ν_{CO} 2102, 2022, 1962, 1930 cm^{-1} (nujol).

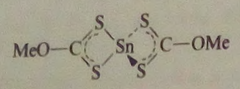
Johnson, B.F.G., *Nature (London)*, 1967, **213**, 901 (*synth, ir*)
Ohyoshi, A. *et al, Chem. Lett.*, 1980, 1537 (*synth, reactions*)

$C_4H_6O_2S_4Sn$ IC-004032

(*O*-Methyl dithiocarbonato)tin

Tin(II) *methylxanthate. Carbonodithioic acid O-methylester, tin(2+) salt (2:1), 9CI. Bis(methylxanthato)tin*(II)

[60671-66-1]



M 333.0
Synth. from $SnCl_2$ + $MeOCS_2K$. Pale yellow cryst. (EtOH/THF). Mp 113-116°.

Ewings, P.F.R. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1399 (*synth, cryst struct*)
Raston, C.L. *et al, Aust. J. Chem.*, 1978, **31**, 1493 (*synth, ir, uv*)

$C_4H_6O_4Pb$ IC-004033

Lead(*II*) acetate

Lead diacetate. Diacetatolead

[301-04-2]

$Pb(OAc)_2$

M 325.2
White cryst. V. sol. H_2O, glycine; v. sl. sol. EtOH. Dec. at 75°.

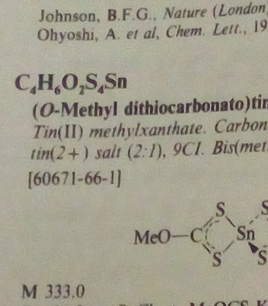
▷ Toxic. AI5250000.

Maciel, G.E. *et al, J. Am. Chem. Soc.*, 1973, **95**, 3039 (*Pb-207 nmr*)
Kharitonova, R.I. *et al, Zh. Neorg. Khim.*, 1975, **20**, 1823 (*synth*)
Gerbeleu, N.V. *et al, Zh. Neorg. Khim.*, 1984, **29**, 1450 (*ms*)
Baraldi, P. *et al, Spectrochim. Acta, Part A*, 1987, **37**, 141 (*ir*)

$C_4H_6O_4Pt$ IC-004034

Platinum(*II*) acetate

[3375-34-6]



tetramer

R = CH_3

M 313.1
Tetrameric.
Tetramer:
$C_{16}H_{24}O_{16}Pt_4$ M 1252.6
Brown plate-like cryst. (HOAc).

[42196-33-8]

Malerbi, B.W., *Chem. Ind. (London)*, 1970, 796 (*synth*)
Carrondo, M.A.A.F. de C.T. *et al, J. Chem. Soc., Chem. Commun.*, 1976, 410 (*tetramer, cryst struct*)

$C_4H_6O_4Sn$ IC-004035

Tin(*II*) acetate

Stannous acetate. Acetic acid, tin(2+) salt, 9CI

[638-39-1]

$Sn(OAc)_2$

M 236.7
Synth. from AcOH + $Sn(OMe)_2$ or bis(methylcyclopentadienyl)tin. Promotes dye uptake by fabrics. Used as a catalyst for e.g. polym. Cryst. Mp 182.5-183°. Bp 240°.

Donaldson, J.D. *et al, J. Chem. Soc.*, 1964, 5942 (*synth*)
Donaldson, J.D. *et al, Spectrochim. Acta*, 1965, **21**, 275 (*ir*)
Ewings, P.F.R. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1717 (*synth, mössbauer*)
Harrison, P.G. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 940 (*synth*)

$C_4H_6O_4Zn$ IC-004036

Zinc acetate ($Zn(OAc)_2$)

[557-34-6]

$Zn(OAc)_2$

M 183.4
Two cryst. forms. α: distorted ZnO_4 tetrahedra; 3D-network with $OAc^{\ominus}$ groups linking two ZnO_4 tetrahedra. β: 2D polymeric sheet of ZnO_4 tetrahedra connected by AcO bridges in a *syn-anti* arrangement. Obt. e.g. from Ac_2O and $Zn(OH)_2$; β-form by dehydration of dihydrate at 236°. Antistatic agent; bactericide; anticorrosion agent; antimicrobial agent; anti-plaque agent; fungicide. Sol. H_2O; org. solvs. except EtOH. Mp 242°. $Subl._{150}$ 200°. Dec. at 180° to $Zn_4O(OAc)_6$.

▷ AK1500000.

Dihydrate: [5970-45-6].
Cryst. (dil. aq. AcOH).
▷ ZG8750000.

Duval, C. *et al, Ann. Phys.*, 1942, **17**, 5 (*uv*)
McCrone, W.C. *et al, Anal. Chem.*, 1949, **21**, 645 (*powder struct, dihydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 980 (*rev, bibl*)
Ananthanarayanan, V., *Proc. Indian. Acad. Sci.*, 1962, **50**, 188 (*raman, dihydrate*)
McAdie, H.G., *J. Inorg. Nucl. Chem.*, 1966, **28**, 2801 (*thermal anal, dihydrate*)
Djega-Mariadassou, G. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **264**, 1753 (*synth, ir, β-form, powder struct*)
Valero Capilla, A. *et al, Cryst. Struct. Commun.*, 1979, **8**, 795 (*cryst struct*)
Panevchik, V.V. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 1373 (*powder struct*)
Baraldi, P. *et al, Spectrochim. Acta, Part A*, 1981, **37**, 89 (*ir, salt and dihydrate*)
Johnson, M.K. *et al, Spectrochim. Acta, Part A*, 1981, **37**, 899 (*raman, ir, salt and dihydrate*)
Marshall, G.L., *Org. Mass Spectrom.*, 1983, **18**, 168 (*ms*)
Caminiti, R. *et al, J. Chem. Phys.*, 1984, **81**, 543 (*cmr, soln struct*)
Clegg, W. *et al, Acta Crystallogr., Sect. C*, 1986, **42**, 1701 (*cryst struct*)
Kunwar, A.C. *et al, J. Magn. Reson.*, 1986, **69**, 124 (*Zn-67 nmr*)
Meier, B.H. *et al, J. Am. Chem. Soc.*, 1987, **109**, 7937 (*cmr*)
Prozarovskaya, Z.N. *et al, Koord. Khim.*, 1988, **14**, 435 (*ir, pmr, dihydrate*)
Tackett, J.E., *Appl. Spectrosc.*, 1989, **43**, 483 (*ir, raman*)

$C_4H_6O_5Ti$ IC-004037

Bis(acetato-*O*)oxotitanium(*IV*), 11CI

Titanium(IV) *diacetate oxide*

[62202-80-6]

$TiO(OAc)_2$

M 181.9
Synth. by refluxing $Ti(OEt)_4$ in acetic anhydride; also synth. by refluxing $TiCl_4$ and HOAc. White solid.
Py complex: [104853-96-5].
$C_9H_{11}NO_5Ti$ M 261.0
Synth. from parent compd. + Py. Pale yellow solid.

Alcock, N.W. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 2238 (*synth*)
Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1986, **25**, 271 (*synth, ir, deriv*)

$C_4H_6O_5Zr$ IC-004038

Bis(acetato-*O*)oxozirconium(*IV*), 11CI

Zirconium acetate oxide ($Zr(OAc)_2O$). Zirconium diacetate oxide. Zirconyl acetate

[5153-24-2]

$ZrO(OAc)_2$

M 225.3
Tetrameric. May be synth. from $Zr(OH)_4$ and AcOH. Commercially available. Many uses ranging from catalysis of lactone polym. and CO/H_2 reactions to antifouling compds., pressure-sensitive adhesive tapes, texturing polyester fibres and improving biaxially stretched polyester film, antimicrobial agents for fabric.
Tetramer: Octakis(acetato)tetraoxotetrazirconium(IV)
$C_{16}H_{24}O_{20}Zr_4$ M 901.2

[20645-04-9]

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **7**, 192; **22**, 793 (*antimicrobial use*)

$C_4H_6O_6U$ IC-004039

Bis(acetato)dioxouranium

Uranyl acetate

$UO_2(OAc)_2$

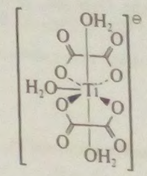
M 388.1
Exists in 5 cryst. modifications. Widely used to detect and determine Li, Na, K, Mg, Zn and other metals forming insol. uranyl acetate compds. Yellow solid. Can be obt. as dihydrate. Forms complexes with donor ligands e.g. R_3PO, R_3AsO.
Dihydrate: [6159-44-0].
$C_4H_{10}O_8U$ M 424.1
Yellow cryst. (AcOH). Sol. H_2O. 7-Coordinate pentagonal bipyramid struct. with 1 H_2O coordinated to U. Ir $\nu_{U=O}$ 949 cm^{-1}. Dehydrates above 80° with slight dec.

Vanino, L., *Chem.-Ztg.*, 1911, **35**, 1005 (*synth*)
Späth, E., *Monatsh. Chem.*, 1912, **33**, 235 (*synth*)
Clough, P.S. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 361 (*tga*)
Mentzen, B. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 1509 (*ir, tga*)
Giorgio, G. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 1517 (*synth, struct*)
Howatson, J. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 1933 (*cryst struct*)

$C_4H_6O_{11}Ti^{\ominus}$ IC-004040

Triaquabis(oxalato)titanate(*III*)(1−)

Triaquabis[ethanedioato(2-)-O,O']titanate(III)(*1−*), *10CI*



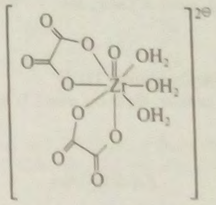
M 277.9 (ion)
Pentagonal bipyramid with H_2O in axial sites.
Cs salt: [65704-09-8].
Synth. by addition of $TiCl_3$ to hot. aq. $H_2C_2O_4$ followed by Cs_2CO_3 and $H_2C_2O_4$. Gold-orange solid.
Cs salt, dihydrate: [64494-64-0].
Formed from anhydrous salt on recryst. from H_2O. Brown solid (H_2O).

Drew, M.G.B. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2919 (*cryst struct, synth, dihydrate*)
Drew, M.G.B. *et al, Inorg. Chim. Acta*, 1977, **25**, L111 (*ir, uv-vis*)

$C_4H_6O_{12}Zr^{2\ominus}$ IC-004041

Triaquabis(oxalato)oxozirconate(*IV*)(2−)

Triaquabis[ethanedioato(2−)-O,O']oxozirconate(IV)(*2−*), *11CI*



M 337.3 (ion)
Geometry not detd.
Ca salt, monohydrate: [97665-29-7].
Synth. from aq. soln. of $CaCl_2$, $ZrOCl_2$ and oxalic acid at pH 1.8-2.0.

Murasé, I., *Ann. Chim. (Paris)*, 1985, **10**, 37 (*synth, thermal dec*)

$C_4H_6S_4Zn$ IC-004042

Bis(dithioacetato)zinc(*II*)

Bis[ethane(dithioato)-S,S']zinc(II), *9CI*

[51637-41-3]

$(H_3CCSS)_2Zn$

M 247.7
Yellow solid (C_6H_6).

Furlani, C. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2404 (*synth, uv*)

$C_4H_7AlO_5$ IC-004043

Aluminium acetate hydroxide ($Al(OAc)_2OH$)

Aluminium hydroxide bis(ethanoate). Bis(acetato-O) hydroxyaluminium

[142-03-0]

$AlOH(OAc)_2$

M 162.0

Synth. from NaOAc and $AlCl_3.6H_2O$ or from $NaAlO_2$ + HOAc. Antiseptic; deodorant; mordant. White solid (H_2O).

Hood, G.C. *et al, J. Am. Chem. Soc.*, 1950, **72**, 2094 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **2**, 102.
Mehrotra, R.C. *et al, Metal Carboxylates*, Academic Press, London, 1983.

IC-004044

$C_4H_7Cl_4NbO_2$

(Butanoato-*O*)tetrachloroniobium(*V*), 11CI

[100072-20-6]

$(H_3CCH_2CH_2COO)NbCl_4$

M 321.8
Synth. from $NbCl_5$ and butanoic acid in 1:1 molar ratio in CCl_4.

Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1985, **24**, 761 (*synth, ir*)

IC-004045

$C_4H_7Cl_4O_2Ta$

(Butanoato-*O*)tetrachlorotantalum(*V*), 11CI

[100072-26-2]

$H_3CCH_2CH_2COOTaCl_4$

M 409.8
Synth. from $TaCl_5$ and Na butanoate. Hygroscopic, yellow-brown solid. Sl. sol. $MeNO_2$, $PhNO_2$, MeCN.

Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1985, **24**, 761 (*synth, ir*)

IC-004046

$C_4H_7FeO_5$

Bis(acetato-*O*)hydroxyiron, 11CI

Basic iron(III) *acetate. Hydroxy iron*(III) *acetate. Basic ferric acetate*

[10450-55-2]

$Fe(OH)(OAc)_2$

M 190.9
Formerly thought to be $Fe(OH)(OAc)_2$. Correctly formulated as acetate salt of Hexakis[μ-(acetato-*O*:*O'*)] triaqua-μ_3-oxotriiron(*III*)(1+), IC-007865.

*Gmelin Handbook Inorg. Chem., Syst. No.*59, 1930, **B4**, 522 (*rev, bibl*)
Dézsi, I. *et al, Chem. Phys. Lett.*, 1973, **22**, 384 (*mössbauer*)
Mahesh, K. *et al, Indian J. Chem., Sect. A*, 1976, **14**, 338 (*mössbauer*)
Catterick, J. *et al, Adv. Inorg. Chem. Radiochem.*, 1977, **20**, 291 (*rev, bibl*)

IC-004047

$C_4H_7N_2NiO_3^{\oplus}$

Glycylglycinatonickel(*II*)(1+), 9CI

[37297-98-6]

$[Ni(H_2NCH_2CONHCH_2CO_2)]^{\oplus}$

M 189.8 (ion)
Simplest Ni(*II*) peptide complex. Formed in soln. Not isol.

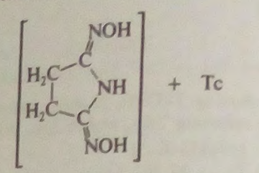
Kim, M.K. *et al, J. Am. Chem. Soc.*, 1967, **89**, 5138 (*uv, ir, props*)
Tipping, E.W. *et al, J. Chem. Soc., Faraday Trans. 1*, 1972, **68**, 1764 (*thermochem*)
Larcher, D. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 2117 (*uv, mcd*)

IC-004048

$[C_4H_7N_3O_2Tc]$

2,5-Pyrrolidinedionedioxime technetium complex

Succinimidedioxime technetium complex



Incomplete formula given; ill-defined cationic complex. Produced by $SnCl_2$ redn. of $TcO_4^{\ominus}$ + ligand; oxidn. state probably Tc^{III}. Yellow.

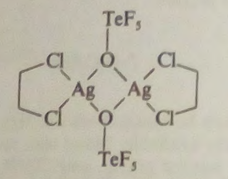
Grases, F. *et al, Radiochim. Acta*, 1986, **40**, 103 (*synth, props*)

IC-004049

$C_4H_8Ag_2Cl_4F_{10}O_2Te_2$

Bis(1,2-dichloroethane-*Cl,Cl'*)bis[μ-[pentafluorohydroxytellurato(1−)-*O*:*O*]]disilver(*I*)

[116887-69-5]



M 890.8
V. moisture-sensitive efflorescent cryst. See also [Pentafluorohydroxytellurato(1−)]silver, IC-000032.

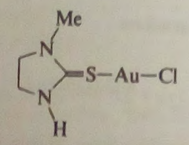
Colsman, M.R. *et al, J. Am. Chem. Soc.*, 1988, **110**, 6886 (*cryst struct, synth, ir, raman, uv*)

IC-004050

$C_4H_8AuClN_2S$

Chloro(1-methyl-2-imidazolidinethione-*S*)gold(*I*), 11CI

[100011-77-6]



M 348.6
Colourless powder (MeOH). Mp 186-187°.

Isab, A.A. *et al, Polyhedron*, 1985, **4**, 1683 (*synth*)

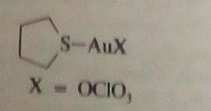
IC-004051

$C_4H_8AuClO_4S$

(Perchlorato-*O*)(tetrahydrothiophene)gold(*I*), 11CI

(Tetrahydrothiophene)gold(1) *perchlorate*

[80330-69-4]



M 384.5
Synth. from $AuCl(SC_4H_8)$ and $AgClO_4$ at −20°. Useful reagent for synth. of organometallic gold(*I*) complexes. Sol. CH_2Cl_2, Et_2O.

▷ Potentially explosive.

Usón, R. *et al, J. Organomet. Chem.*, 1981, **218**, 265 (*synth, reactions*)

C_4H_8AuClS

Chloro(tetrahydrothiophene)gold(*I*)

[39929-21-0]

As (Perchlorato-*O*)(tetrahydrothiophene)gold(*I*), IC-004051 with

X = Cl

M 320.5
Possesses antiarthritic activity. V. useful intermed. for synth. of co-ordination compounds and organometallics. Colourless cryst. (EtOH). Thermally unstable. Mp 109° dec.

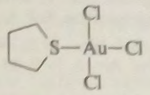
Allen, E.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 2257 (*ir, raman*)
Usón, R. *et al, J. Organomet. Chem.*, 1977, **131**, 471 (*synth*)
U.S. Pat., 4 112 113, (1977); 1979, **90**, 127542s (*synth, antiarthritic activity*)

IC-004053

$C_4H_8AuCl_3S$

Trichloro(tetrahydrothiophene)gold(*III*)

[29991-21-7]



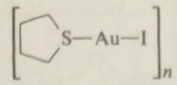
M 391.4
V. useful intermed. for forming Au(*III*) complexes.

Ray, P.C. *et al, J. Indian Chem. Soc.*, 1930, **1**, 67 (*synth*)
Allen, E.A. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 2257 (*synth, ir, raman*)
Usón, R. *et al, Inorg. Chim. Acta*, 1981, **52**, 29 (*reactions*)

IC-004054

C_4H_8AuIS

Iodo(tetrahydrothiophene)gold(*I*)



M 412.0
Exists as dimeric polymer consisting of zig-zag infinite chain of AuI_2 and $Au(SC_4H_8)_2$ linear fragments linked by short Au—Au contacts of 297-298 pm.

Dimer: [95344-34-6]. *Diiodobis(tetrahydrothiophene)digold homopolymer, 11CI*
$C_8H_{16}Au_2I_2S_2$ M 824.0
Light yellow prismatic cryst.

Ahrland, S. *et al, Inorg. Chem.*, 1985, **24**, 1330 (*synth, cryst struct*)

IC-004055

$C_4H_8AuNO_2S$

(Methyl-L-cysteinato-*N,S*)gold, 11CI

[93095-16-0]

$[AuSCH_2CH(NH_2)COOMe]_n$

M 331.1
Polymeric. Colourless cryst. Insol. all common solvs.

Ambach, E. *et al, Z. Naturforsch., B*, 1984, **39**, 1129 (*synth*)

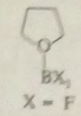
IC-004056

$C_4H_8BF_3O$

Trifluoro(tetrahydrofuran)boron, 10CI

Tetrahydrofuran compd. with trifluoroborane (1:1), 9CI. Tetrahydrofuran compd. with boron fluoride (BF_3) (1:1), 8CI. Trifluoroborane tetrahydrofuran

[462-34-0]



M 139.9
Catalyst. Moisture-sensitive white solid or colourless liq. Mp 12°.

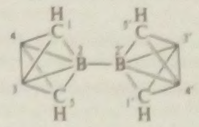
McLaughlin, D.E. *et al, J. Am. Chem. Soc.*, 1960, **82**, 5621 (*pmr*)
Begun, G.M. *et al, J. Chem. Phys.*, 1963, **38**, 2112 (*raman, ir*)
Fratiello, A. *et al, Inorg. Chem.*, 1969, **8**, 480 (*pmr*)
Krysin, A.P. *et al, Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1977, 151.
Hui, B.C., *Inorg. Chem.*, 1980, **19**, 3185 (*use*)
Grinevich, T.V. *et al, Vysokomol. Soedin., Ser. A*, 1980, **22**, 1576 (*use*)

IC-004057

$C_4H_8B_6$

2,2'-Bi-1,5-dicarbapentaborane(5)

[60569-26-8]



M 120.9
Synth. by polym. of 1,5-$C_2B_3H_5$ or from $PtBr_2$ + 1,5-$C_2B_3H_5$ at r.t. Colourless liq. (by dist.). Sol. hexane. V.p. 6 mm at 0°.

Burg, A.P. *et al, Inorg. Chem.*, 1972, **11**, 1962 (*synth*)
Fehlner, T.P. *et al, J. Am. Chem. Soc.*, 1980, **102**, 2644 (*synth, B-11 nmr, pmr, ms, ir, raman*)
Sneddon, L.G. *et al, J. Am. Chem. Soc.*, 1984, **106**, 2275, 7793 (*synth, B-11 nmr, pmr, ir, ms*)

IC-004058

$C_4H_8Br_4CrO_4^{2\ominus}$

Bis(acetic acid)tetrabromochromate(*II*)(2−)

$[CrBr_4(HOAc)_2]^{2\ominus}$

M 491.7 (ion)
Distorted octahedral anion. Apparently incorrectly indexed in 11CI.

trans-form
Interatomic distances: Cr—Br 263.7, 283.9; Cr—O 206 pm.

Bis-guanidinium salt: [77135-55-8].
Synth. from guanidinium bromide + $CrBr_3$ in AcOH. Air-sensitive light green cryst. (AcOH). High spin complex.

[87196-97-2]

Babar, M.A. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 27 (*synth, magnetism, uv*)
Babar, M.A. *et al, J. Crystallogr. Spectrosc. Res.*, 1983, **13**, 325 (*cryst struct*)

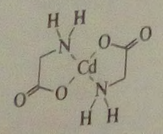
IC-004059

$C_4H_8CdN_2O_4$

Bis(glycinato-*N,O*)cadmium

Cadmium glycinate

[14376-36-4]



M 260.5

Prepd. from CdO + glycine in H_2O. Cryst. + $1H_2O$ (H_2O).

Low, B.W. *et al, J. Am. Chem. Soc.*, 1959, **81**, 4412 (*synth, cryst struct*)
Krishnan, K. *et al, Inorg. Chem.*, 1967, **6**, 55 (*raman*)
Ashby, C.I.H. *et al, J. Am. Chem. Soc.*, 1980, **102**, 2990 (*nqr*)
Matsui, H., *J. Inorg. Nucl. Chem.*, 1981, **43**, 2187 (*stability const*)

IC-004060

$C_4H_8CdN_6S_2Se_2$

Bis(selenourea-*Se*)bis(thiocyanato-*N*)cadmium

Bis(isothiocyanato)bis(selenourea-Se)*cadmium*(II). *Bis(selenourea)cadmium bis(isothiocyanate). Cadmium*(II) *thiocyanate bis(selenourea)*

[28604-26-4]

$[(H_2N)_2C{=}Se]_2Cd(NCS)_2$

M 474.6

Polymeric struct. with octahedral Cd. Isostructural with corresp. (thiourea)nickel complex. Cryst.

Domiano, P. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 591 (*powder struct, ir*)

IC-004061

$C_4H_8CdN_6S_4$

Bis(thiocyanato-*N*)bis(thiourea-*S*)cadmium(*II*)

Bis(isothiocyanato)bis(thiourea-S)*cadmium*(II). *Cadmium*(II) *isothiocyanate bis(thiourea)*

[28604-25-3]

$[(H_2N)_2C{=}S]_2Cd(NCS)_2$

M 380.8

Polymeric struct. with octahedral Cd. Needles.

[29893-48-9]

Domiano, P. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 591 (*powder struct, ir*)
Flint, C.D. *et al, Inorg. Chem.*, 1969, **8**, 1833 (*synth, ir*)
Selvarajan, A., *Indian J. Pure Appl. Phys.*, 1970, **8**, 338 (*ir, raman*)

IC-004062

$C_4H_8Cl_2CrO$

Dichloro(tetrahydrofuran)chromium(*II*), 11Cl, 10Cl, 9Cl

Chromium(II) *chloride tetrahydrofuran*

[52721-12-7]

$[CrCl_2(THF)]_n$

M 195.0

Prob. chloride-bridged polymer with distorted octahedral chromium. Synth. by treating Cr pellets with dry HCl gas in pure THF under N_2. V. useful starting material in non-aqueous synth. White air-sensitive solid. Also known are $CrCl_2(THF)_3$ and $CrBr_2(THF)_2$.

[36463-97-5]

Larkworthy, L.F. *et al, Chem. Ind. (London)*, 1974, 164 (*synth, uv-vis*)
Girolami, G.S. *et al, J. Am. Chem. Soc.*, 1983, **105**, 5954 (*use*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 717, 739 (*rev*)

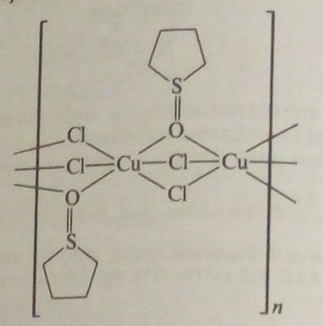
IC-004063

$C_4H_8Cl_2CuOS$

Dichloro(tetrahydrothiophene 1-oxide-*O*)copper, 11Cl

Copper(II) *chloride tetramethylene sulfoxide*

[66690-14-0]



M 238.6

Cu...Cu 320.9 pm. Coordination severely distorted from octahedral with 4 short bonds and 2 long bonds. Ferromagnetic linear chains. Synth. by addn. of anhydr. $CuCl_2$ to a 1-propanol soln. of tetramethylene sulfoxide at 70°. Thin orange needles. Sol. hot 1-propanol.

Willett, R.D. *et al, J. Appl. Phys.*, 1978, **49**, 1329 (*magnetism*)
Swank, D.W. *et al, Phys. Rev. B*, 1979, **20**, 2154 (*cryst struct, synth*)
Landee, C.P. *et al, J. Appl. Phys.*, 1982, **53**, 1888 (*magnetism*)
Bosch, L.A. *et al, J. Phys. C*, 1987, **20**, 2307 (*magnetism*)

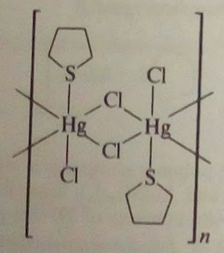
IC-004064

$C_4H_8Cl_2HgS$

Dichloro(tetrahydrothiophene)mercury(*II*)

(Tetrahydrothiophene)mercury dichloride. Di-μ-chlorodichlorobis(tetrahydrothiophene)dimercury

[24593-06-4]



M 359.6

Polymeric in solid state with infinite double chains. Needles (Me_2CO). Mp 129-130°.

[25426-34-0]

Whitehead, E.V. *et al, J. Am. Chem. Soc.*, 1951, **73**, 3632.
Parham, W.E. *et al, J. Am. Chem. Soc.*, 1959, **81**, 6071 (*synth*)
Brändén, C.I., *Ark. Kemi.*, 1964, **22**, 495 (*cryst struct*)
Biscarini, P. *et al, J. Chem. Soc. A*, 1969, 2206 (*synth, ir*)
Farhangi, Y. *et al, Aust. J. Chem.*, 1973, **26**, 983 (*heat of formn, formn const*)

IC-004065

$C_4H_8Cl_2MnO_2$

Dichloro(1,4-dioxane)manganese(*II*), 9Cl

Manganese(II) *chloride 1,4-dioxane*

[26613-91-2]

$MnCl_2$(dioxan)

M 213.9

Polymeric layer struct. with octahedral Mn surrounded by 4Cl (equatorial) and 2O (axial). Prepd. from dioxane and $MnCl_2$. Colourless cryst., not hygroscopic. V. sol. H_2O, EtOH. $\mu_{eff} = 5.88\mu_B$ (292K).

Dihydrate:

$C_4H_{12}Cl_2MnO_4$ M 249.9

Prepd. from $MnCl_2.4H_2O$ in EtOH and dioxane. Bright pink cryst.

Osthoff, R.C. *et al, J. Am. Chem. Soc.*, 1954, **76**, 4732 (*synth*)
Fowles, G.W.A., *J. Chem. Soc. A*, 1968, 1842 (*synth, cryst struct, ir, uv, magnetism*)
Barnes, J.C. *et al, J. Chem. Soc. A*, 1970, 1442 (*struct, thermal anal, ir, hydrate*)
Fowles, G.W.A. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 143 (*ir*)
Chaudhuri, N.R. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 2375 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 152 (*rev, bibl*)

IC-004066

$C_4H_8Cl_3FeO$

Trichloro(tetrahydrofuran)iron

Iron(III) *chloride THF solvate*

[36470-52-7]

$FeCl_3(THF)$

M 234.3

Convenient source of Fe(*III*). Couples with Grignard reagents. Moisture sensitive golden yellow cryst. Sol. THF, C_6H_6, 1,2-dichloroethane; sl. sol. $PhNO_2$, $CHCl_3$; insol. CCl_4, cyclohexane. $Subl._{0.45}$ 80-85°. $\mu_{eff} = 5.79\mu_B$.

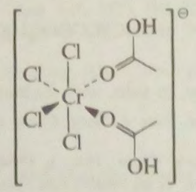
Benner, L.S. *et al, Inorg. Chem.*, 1972, **11**, 652 (*synth, ir, uv*)
Ger. Pat., 2 542 489, (1976); *CA*, **85**, 47530 (*use*)
Cotton, F.A. *et al, Acta Crystallogr., Sect. C*, 1990, **46**, 1424 (*cryst struct*)

IC-004067

$C_4H_8Cl_4CrO_4^{\ominus}$

Bis(acetic acid)tetrachlorochromate(*III*)(1 –)

Bis(acetato-O)*tetrachlorochromate*(III)(*3* –), *dihydrogen, 10Cl*



M 313.9 (ion)

cis-Config. suggested by spectra.

cis-form

Et_4N salt: [67253-17-2].
Bright purple cryst.

Quinolinium salt: [67253-20-7].
Bright purple powder.

[61567-25-7, 61567-27-9]

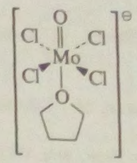
Seddon, K.R. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2195 (*synth, ir, uv-vis*)

IC-004068

$C_4H_8Cl_4MoO_2^{\ominus}$

Tetrachlorooxo(tetrahydrofuran)molybdate(*V*)(1 –), 11Cl, 10Cl

[67588-63-0]



M 325.8 (ion)

trans-Octahedral anion. Interatomic distances: Mo=O 167.3, Mo—O_{THF} 235.6, Mo—Cl_{av} 239.0 pm (corrected values).

Hexakis(tetrahydrofuran)magnesium(2+) salt (2:1): [102578-94-9].
Air-sensitive green cryst. Sol. CH_2Cl_2. Ir ν_{MoO} 990 cm^{-1}. Paramagnetic; $\mu_{eff} = 1.70\mu_B$ (298K).

Tri-μ-chlorohexakis(tetrahydrofuran)dimagnesium(1+) salt (1:1): [102604-55-7].
Green cryst. Ir ν_{MoO} 980 cm^{-1}.

1,4-Bis(1-oxa-4,10-dithia-7H-7-azoniacyclodecan-7-ylmethyl) benzene(2+) salt, (2:1): [79549-06-7].
Green cryst. (MeCN/THF).

Bird, P.H. *et al, Can. J. Chem.*, 1981, **59**, 2879 (*synth, cryst struct*)
Sobota, P. *et al, Z. Anorg. Allg. Chem.*, 1986, **533**, 215 (*cryst struct, Mg, salts, synth, ir*)

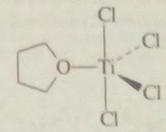
IC-004069

$C_4H_8Cl_4OTi$

Tetrachloro(tetrahydrofuran)titanium(*IV*), 11Cl

Titanium(IV) *chloride tetrahydrofuran*

[15005-09-1]



M 261.7

Synth. by adding excess $TiCl_4$ to THF in toluene or CH_2Cl_2. Catalyses polym. of ethylene. Dark yellow solid. Mp 138-139° dec.

Hamilton, P.M. *et al, J. Am. Chem. Soc.*, 1953, **75**, 2881 (*synth*)
Perkins, P.G. *et al, J. Chem. Soc. A*, 1970, 3229 (*synth, thermochem*)
Eur. Pat., 11 308, (1980); *CA*, **94**, 31309c (*use*)
Ikonitskii, I.V. *et al, Zh. Prikl. Spektrosk.*, 1981, **34**, 673; *CA*, **94**, 216795b (*ir*)

IC-004070

$C_4H_8Cl_5OTi^{\ominus}$

Pentachloro(tetrahydrofuran)titanate(*IV*)(1 –), 11Cl

$[Cl_5Ti(THF)]^{\ominus}$

M 297.2 (ion)

Octahedral anion.

Tri-μ-chlorohexakis(tetrahydrofuran)dimagnesium(1+) salt: [94081-80-8].
$C_{28}H_{56}Cl_8Mg_2O_7Ti$ M 884.8
Synth. by direct reaction of $TiCl_4(THF)_2$ and $MgCl_2(THF)_2$ in THF. Air-sensitive yellow solid (THF).

Sobota, P. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2077 (*synth, cryst struct*)
Sobota, P., *Proc. Conf. Coord. Chem., 10th*, 1985, 357; *CA*, **104**, 236209s (*reactions*)

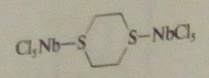
IC-004071

$C_4H_8Cl_{10}Nb_2S_2$

Decachloro[μ-(1,4-dithiane-S^1:S^4)]diniobium(*IV*), 11Cl

Niobium(V) chloride hemi-(1,4-dithiane) complex

[57937-19-6]



M 660.5

Synth. by adding a soln. of 1,4-dithiane in CH_2Cl_2 to $NbCl_5$. Red solid.

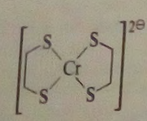
Wade, S.R. *et al, Inorg. Chim. Acta*, 1983, **72**, 201 (*synth, ir, pmr*)

IC-004072

$C_4H_8CrS_4^{2\ominus}$

Bis[1,2-ethanedithiolato(2−)-*S,S*']chromate(*III*)(2−), 11Cl

[94750-79-5]



M 236.3 (ion)

Planar anion, unusual stereochem. for Cr(*III*); Cr—S 238.8 pm. μ_{eff} = 4.95μ_B (297K, MeCN).

Bis-Et$_4$N salt: [94750-80-8].

Violet, air-sensitive cryst. (MeCN/Et_2O).

Rao, C.P.R. *et al, Inorg. Chem.*, 1986, **25**, 428 (*cryst struct*)
Mukherjee, R.N. *et al, Inorg. Chem.*, 1986, **25**, 2979 (*electrochem, uv*)

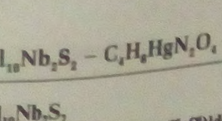
IC-004073

$C_4H_8CuN_2O_2S_2$

Fluopsin C

Bis(N-hydroxy-N-methylmethanethioamidato-O,S)copper, 9Cl. Bis(N-methylthioformohydroxamato)copper, 8Cl. YC 73. Antibiotic YC 73

[31323-25-8]



M 243.7

Isol. from *Pseudomonas fluorescens*. Possesses antibacterial props. Dark-green cryst. (EtOH). Mp 199° dec. λ_{max} 231, 253, 267, 320 and 365 nm (MeOH).

▷ GL6490000.

Shirahata, K. *et al, J. Antibiot.*, 1970, **23**, 546 (*isol, struct*)
Egawa, Y. *et al, J. Antibiot.*, 1971, **24**, 124 (*struct, synth*)
Shirahata, K. *et al, J. Antibiot.*, 1971, **24**, 140 (*synth, ir, nmr*)
Taylor, D., *Cryst. Struct. Commun.*, 1978, **7**, 237 (*cryst struct*)
Bell, S.J. *et al, Antimicrob. Agents Chemother.*, 1979, **15**, 384 (*props*)

IC-004074

$C_4H_8CuN_2O_4$

Bis(glycinato)copper, 11Cl, 10Cl, 9Cl, 8Cl

[13479-54-4]

cis-form

M 211.6

Used in photometric detn. of Cu and in catalysis.

cis-form [10171-08-1]

Monohydrate: [23678-02-6].

Dark blue needles.

trans-form [10170-99-7]

Monohydrate: [14932-09-3].

Deep blue rhombic cryst. Sol. H_2O, sl. sol. EtOH. Mp 228° dec.

Dihydrate: [23678-01-5].

Light blue powdery cryst. Sol. H_2O. Mp 225° dec.

Tomita, V.K., *Bull. Chem. Soc. Jpn.*, 1961, **34**, 280 (*cryst struct, synth*)
Herlinger, A.W. *et al, J. Am. Chem. Soc.*, 1970, **92**, 6474 (*ir*)
Allen, H.C. *et al, J. Chem. Phys.*, 1972, **56**, 997 (*esr*)
Hayakawa, K. *et al, Bull. Chem. Soc. Jpn.*, 1973, **46**, 2792 (*use*)
Rupp, H. *et al, Bioinorg. Chem.*, 1976, **6**, 45 (*pe*)
O'Brien, P., *J. Chem. Educ.*, 1982, **59**, 1052 (*synth, ir*)
Merck Index, 11th Ed., 1989, No. 2644.

IC-004075

$C_4H_8HgN_2O_2$

Bis(acetamidato)mercury

Mercuric acetamide

[26370-40-1]

$H_3CCONH\text{-}Hg\text{-}NHCOCH_3$ (soln. struct.)

M 316.7

Mercurating agent. Cryst. (MeOH or EtOH); dec. on standing → acetamide and $[HgNAc]_n$; dec. similarly in soln. Sol. MeOH/Me_2CO. Mp 201-203° dec. (195°).

Kahovec, L. *et al, Z. Phys. Chem.* (*Leipzig*), 1941, **51**, 49 (*synth, raman*)
Williams, J.W. *et al, J. Am. Chem. Soc.*, 1942, **64**, 1738 (*synth*)
Kutzelnigg, W. *et al, Spectrochim. Acta*, 1962, **18**, 549 (*ir*)
Kamenar, B. *et al, Inorg. Chim. Acta*, 1969, **3**, 25 (*cryst struct*)
Brown, D.B. *et al, Inorg. Chim. Acta*, 1969, **3**, 644 (*synth, pmr*)

IC-004076

$C_4H_8HgN_2O_4$

Bis(glycinato)mercury(*II*)

Mercury glycinate

[15283-87-1]

$(H_2NCH_2COO)_2Hg$

M 348.7

Synth in soln. Dec. in soln. with formation of Hg.

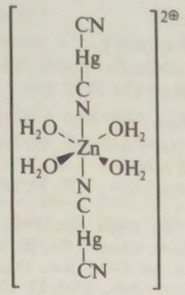
Toropova, V.F. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1966, **11**, 288.
Long, T.V. *et al, Inorg. Chem.*, 1967, **6**, 1754 (*raman*)
Van der Linden, W.E. *et al, Anal. Chim. Acta*, 1974, **68**, 143 (*stability const*)
Van der Linden, W.E. *et al, Talanta*, 1975, **22**, 89 (*stability const*)
Reid, R.S. *et al, J. Inorg. Biochem.*, 1988, **32**, 183 (*pmr*)

IC-004077

$C_4H_8Hg_2N_4O_4Zn^{2\oplus}$

Bis[μ-(cyano-*C*:*N*)]bis(cyano-*C*)(tetraaquazinc) dimercury(2+), 9Cl

Tetraaquadi-μ-cyanodicyanozincdimercury(2+)



M 642.7 (ion)

trans-Octahedral in solid state.

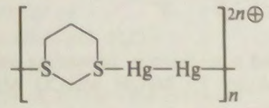
Dinitrate: Synth. from $Zn(NO_3)_2$ + $Hg(CN)_2$ in H_2O. Cryst. + $3H_2O$.

Nylander, C.W.G., *J. Prakt. Chem.*, 1860, **79**, 379.
Mahon, C., *Inorg. Chem.*, 1971, **10**, 1813 (*synth, ir, cryst struct*)
Power, A.F. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 2072 (*nd*)

IC-004078

$C_4H_8Hg_2S_2^{2\oplus}$

[μ-(1,3-Dithiane)]dimercury(*I*)(2+)



M 521.4 (ion)

In dinitrate salt, $NO_3^{\ominus}$ units link the $C_4H_8S_2Hg_2^{2\oplus}$ chains.

Dinitrate: [80694-43-5].

Cryst. (MeOH). Mp 150° dec.

[58168-89-1]

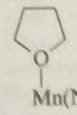
Brodersen, K. *et al, Chem. Ber.*, 1975, **108**, 3243 (*synth, ir*)
Brodersen, K. *et al, Z. Anorg. Allg. Chem.*, 1977, **428**, 166 (*cryst struct*)
Brodersen, K. *et al, Z. Anorg. Allg. Chem.*, 1981, **482**, 217 (*synth, raman*)

IC-004079

$C_4H_8MnN_3O_4$

Trinitrosyl(tetrahydrofuran)manganese, 11Cl

[56315-56-1]



M 217.0

Synth. by photolysis of a THF soln. of $Mn_2(CO)_{10}$ saturated with NO. Useful intermed. for the synth. of the complexes $Mn(NO)_3L$ (L = PR_3, AsR_3, 1,2-di-2-pyridylethylene). Almost opaque olive green soln. in THF which can be stored for at least 2 months at −10° under N_2.

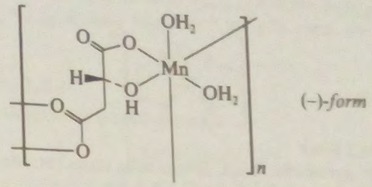
Herberhold, M. *et al, J. Organomet. Chem.*, 1974, **67**, 81 (*synth, ir*)
Wilson, R.D. *et al, J. Organomet. Chem.*, 1980, **191**, 123 (*synth, ir*)

IC-004080

$C_4H_8MnO_7$

Diaquabis[hydroxybutanedioato(1−)]manganese(*II*)

Diaqua(malato)manganese(II)



(−)-*form*

M 223.0

Polymeric chain struct. with octahedral Mn.

(−)-*form* [56994-99-1]

Synth. from $MnCO_3$ and *S*-malic acid in H_2O. Colourless cryst. (H_2O).

Karipides, A. *et al, Inorg. Chem.*, 1976, **15**, 44 (*synth, cryst struct*)

IC-004081

$C_4H_8MnO_8$

Diaqua[2,3-dihydroxybutanedioato(2−)-O^1,O^2] manganese(*II*), 11Cl

Diaqua(μ-+L-tartrato)manganese(II)

[13001-56-4]

$Mn(OH_2)_2(OOCCHOHCHOHCOO)$

M 239.0

Polymeric struct. with v. distorted octahedral Mn (as dihydrate). Synth. from $MnCl_2$ or $MnSO_4$ with $K_2C_4H_4O_6$ in H_2O. Pink cryst.

Dihydrate: [102532-45-6].

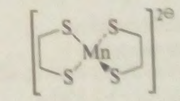
Synth. by slow evaporation of an aq. soln. of tartaric acid and $MnCl_2$ at r.t. Blue-green prisms.

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, D2, 170 (*rev, bibl*)
Soylu, H., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1985, **171**, 255 (*synth, cryst struct*)

IC-004082

$C_4H_8MnS_4^{2\ominus}$

Bis(1,2-ethanedithiolato)manganate(*II*)(2−)



M 239.3 (ion)

Tetrahedral anion, Mn—S 243 pm (mean). Yellow-green anion (MeCN). μ_{eff} = 5.06μ_B (MeCN).

Bis-Me_4N salt: [87860-05-7].

Synth. from $MnCl_2$ and $NaSCH_2CH_2SNa$ in MeOH and stoichiometric amounts of $[Me_4N]Cl$ under N_2. Yellow cryst. + $\frac{1}{2}$MeCN (MeCN). Insol. Et_2O.

Bis-Ph_4P salt: [87860-06-8].

Synth. from $MnCl_2$, $NaSCH_2CH_2SNa$, $[Ph_4P]Cl$ in MeOH under N_2. Orange-yellow cryst. μ_{eff} = 6.02μ_B (298K).

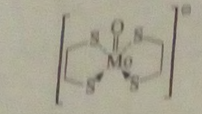
Costa, T. *et al, Inorg. Chem.*, 1983, **22**, 4091 (*synth, cryst struct, magnetism, uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, D7, 38 (*rev, bibl*)

IC-004083

$C_4H_8MoOS_3^{\ominus}$

Bis(ethane-1,2-dithiolato-*S,S'*)oxomolybdate(*IV*)

Bis[1,2-ethanedithiolato(2−)-S,S']oxomolybdate(V) (1−),11Cl



M 296.3 (ion)
Square pyramidal struct. Interatomic distances: Mo=O 167.8, Mo—S 237.2, S—C 176.0 pm.

Ph_4P salt: [106708-03-6].
Black cryst. (CH_2Cl_2/Et_2O).

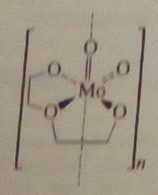
Ellis, S.R. *et al, J. Chem. Soc., Chem. Commun.*, 1986, 1483 (*cryst struct, synth, esr*)

IC-004084

$C_4H_8MoO_5$

Dioxo[2,2'-oxybis[ethanolato]](2−)-*O,O',O'']molybdenum(*VI*), 11Cl

[73440-38-7]



M 232.0

cis-form [85047-93-4]
Octahedral, with asymmetric Mo—O bridge forming polymeric chain struct. Synth. from MoO_3 and ligand. Cryst.

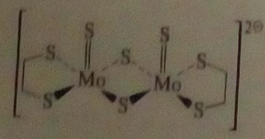
Knobler, C. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 248 (*synth, ir*)
Wilson, A.J. *et al, Acta Crystallogr., Sect. C*, 1983, **39**, 329 (*synth, cryst struct*)

IC-004085

$C_4H_8Mo_2S_8^{2\ominus}$

Bis(ethylene-1,2-dithiolato)di-μ-sulfidodisulfidodimolybdate(2−)

Di-μ-sulfidobis[(ethylene-1,2-dithiolato)sulfidomolybdate(V)]
Bis[1,2-ethanedithiolato(2−)-S,S']di-μ-thioxodithioxodimolybdate(2−), 11Cl, 10Cl. (*Ethane-1,2-dithiolato-S,S')bis(μ-sulfido)disulfidodimolybdate(V)(2−)*
[64582-89-4]



syn-form

M 504.5 (ion)
Tetragonal-pyramidal molybdenum. First example of *syn* and *anti* isomerism in di-μ-sulfido-bridged Mo^V complex.

syn-form [65137-00-0]
cis-form
Non-planar Mo_2S_4 core.

Bis-Et_3NH salt: [96647-87-9].
Dark brown cryst. Mo—Mo 285.5 pm.

Bis-Et_4N salt: [65137-01-1].
Red-violet prisms. Sol. MeCN. Diamagnetic; Mo—Mo 286.3 pm.

anti-form [65045-65-0]
trans-form
Planar Mo_2S_2 core.

Bis-Et_4N salt: [65045-66-1].
Red-violet rhombohedral plates. Sol. MeCN. Diamagnetic; Mo—Mo 287.8 pm.

[63447-81-4, 63447-82-5, 63699-87-6, 63699-88-7, 92763-40-1]

Bunzey, G. *et al, J. Am. Chem. Soc.*, 1977, **99**, 417, 4168 (*props, ir, synth, cryst struct, isomers*)
Bunzey, G. *et al, Inorg. Chem.*, 1978, **17**, 682 (*cryst struct, ir, electrochem*)
Miller, K.F. *et al, J. Am. Chem. Soc.*, 1980, **102**, 5102 (*synth, ir*)
Chandler, T. *et al, Inorg. Chem.*, 1981, **20**, 75.
Halbert, T.R. *et al, J. Am. Chem. Soc.*, 1983, **105**, 5476 (*syn form*)
Pan, W.-H. *et al, Inorg. Chem.*, 1984, **23**, 4265; 1983, **22**, 672.
Hsieh, T.C. *et al, Transition Met. Chem.*, 1985, **10**, 81 (*cryst struct, syn-form, synth*)

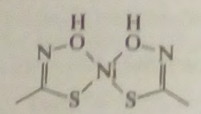
IC-004086

$C_4H_8N_2NiO_2S_2$

Bis(thioacetohydroxamato)nickel

Bis(methylthiohydroxamato)nickel(II)

[15790-75-7]



cis-form

M 238.9
Obt. as *cis*, and *trans*-isomers, depending on recryst. solv. Brown solid. Sol. Py, MeOH, Me_2CO. Mp >280°. Diamagnetic.

[23740-04-7]

Sato, T. *et al, J. Chem. Soc., Chem. Commun.*, 1966, 192; 1967, 215 (*synth, cryst struct*)
Nagata, K. *et al, Chem. Pharm. Bull.*, 1967, **15**, 61, 70 (*synth, ir, uv-vis*)
Sato, T. *et al, J. Chem. Soc. B*, 1968, 989; 1969, 125.

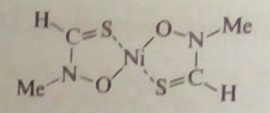
IC-004087

$C_4H_8N_2NiO_2S_2$

Fluopsin N

Bis(N-*hydroxy*-N-*methylmethanethioamidato*-O,S)*nickel, 9Cl*

[31541-90-9]



M 238.9
Isol. from *Pseudomonas fluorescens*. Antibiotic props. resemble those of Fluopsin B, IC-005134. Purple cryst.

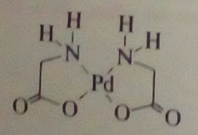
Japan. Pat., 73 10 554, (1973); *CA*, **80**, 35824 (*synth*)
Leong, J. *et al, Inorg. Chem.*, 1978, **17**, 1886 (*synth, nmr*)
Bell, S.J. *et al, Antimicrob. Agents Chemother.*, 1979, **15**, 384 (*props*)

IC-004088

$C_4H_8N_2O_4Pd$

Bis(glycinato)palladium(*II*)

[14592-68-8]



cis-form

M 254.5
Square planar.

cis-form [14281-81-3]
Prepd. by heating glycine + K_2PdCl_4 in H_2O. Pale yellow needles.

trans-form [23678-00-4]
Prepd. from glycine + K_2PdCl_4 in H_2O at r.t. Pale yellow plates.

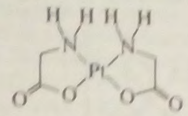
[71580-78-4]

Coe, J.S., *J. Chem. Soc. A*, 1971, 829 (*synth, ir*)
Boradenko, V.S. *et al, Zh. Strukt. Khim.*, 1976, **17**, 479 (*pmr*)
Shchelokov, A.Yu. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1977, **22**, 3303 (*raman*)
Shestakova, N.A. *et al, Koord. Khim.*, 1978, **4**, 587 (*synth*)
Baidina, I.A. *et al, Zh. Strukt. Khim.*, 1979, **20**, 544; 1982, **23**, 88 (*cryst struct*)

IC-004089

$C_4H_8N_2O_4Pt$

Bis(glycinato)platinum(*II*), 8Cl



cis-form

M 343.1
Both isomers known, photochemically interconverted.

cis-form
Yellow cryst. Sol. H_2O.

trans-form [14592-69-9]
Colourless solid. Sol. H_2O.

[14592-69-9, 15685-00-4]

Pinkard, F.W. *et al, J. Chem. Soc.*, 1934, 1012 (*synth*)
Scandola, F. *et al, Inorg. Chim. Acta*, 1967, **1**, 76 (*synth*)
Freeman, H.C. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 1203 (*struct, trans-form*)
Webb, D.L. *et al, Inorg. Chem.*, 1971, **10**, 2213 (*uv-vis, fluorescence*)
Pozhidaev, A.I. *et al, J. Struct. Chem. USSR* (*Engl. Transl.*), 1975, **16**, 997 (*struct, cis-form*)
Kharitonov, Yu.Ya. *et al, Z. Naturforsch., B*, 1982, **37**, 1034 (*ir*)

IC-004090

$C_4H_8N_2O_4Zn$

Bis(glycinato)zinc

Zinc glycinate

[14281-83-5]

$$Zn(H_2NCH_2COO)_2$$

M 213.5
Prepd. from ZnO + glycine in boiling H_2O. Cryst. + H_2O (H_2O or aq. EtOH). Sol. H_2O. Mp 319° dec.

[28678-61-7]

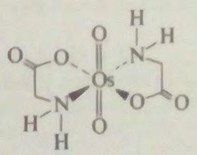
Low, B.W. *et al, J. Am. Chem. Soc.*, 1959, **81**, 4412 (*synth, cryst struct, hydrate*)
Nakamoto, K. *et al, J. Am. Chem. Soc.*, 1961, **83**, 4528 (*ir*)
Krishnan, K. *et al, Inorg. Chem.*, 1967, **6**, 55 (*raman*)

IC-004091

$C_4H_8N_2O_6Os$

Bis(glycinato)dioxoosmium(*VI*)

[77153-90-3]



M 370.3
All *trans*-octahedral. Synth. from OsO_4 and glycine in H_2O, crysts. form v. slowly. Brightly coloured needles. Dec. in common solvs. Ir $\nu_{Os=O}$ 850 cm^{-1}.

Roth, W.J. *et al, Inorg. Chem.*, 1981, **20**, 2023 (*synth, cryst struct, ir*)

IC-004092

$C_4H_8N_4O_4Zn^{2\ominus}$

Tetrakis(formamidato)zincate(2−)

$$[Zn(NHC(O)H)_4]^{2\ominus}$$

M 241.5 (ion)
Di-Na salt: [30927-58-3].
Synth. *in situ*, not isol. Sol. formamide.
Di-K salt: [30927-59-4].
Synth. *in situ*, not isol. Sol. formamide.

Paul, R.C. *et al, Indian J. Chem.*, 1970, **8**, 939 (*synth, props*)

IC-004093

$C_4H_8N_6NiS_4$

Bis(thiocyanato-*S*)bis(thiourea-*S*)nickel, 10Cl

Dithiocyanatobis(thiourea)nickel(II)

[28604-23-1]

$$(NCS)_2Ni[S{=}C(NH_2)_2]_2$$

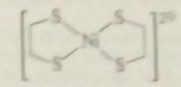
M 327.1
6-Coordinate Ni, bound to two NCS via N, and four S in polymeric struct. Green prismatic cryst. (amyl alcohol). Sol. EtOH; sl. sol. Py (with dec.). Mp 225°. μ_{eff} = 2.87 μ_B.

Yamaguchi, A. *et al, J. Am. Chem. Soc.*, 1958, **80**, 527.
Olliff, R.W., *J. Chem. Soc.*, 1965, 2036.
Nardelli, M. *et al, Acta Crystallogr.*, 1966, **20**, 349 (*cryst struct*)
Patel, R.N. *et al, Indian J. Chem.*, 1966, **4**, 44 (*synth, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1968, **C2**, 1016 (*rev*)

IC-004094

$C_4H_8NiS_4^{2\ominus}$

Bis(1,2-ethanedithiolato-*S,S'*)nickelate(*II*)(2−)



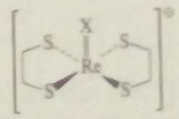
M 243.0 (ion)
Formed from $NiCl_2$ and 1,2-ethanedithiol. Formed in soln. Not isol.

Leussing, D.L. *et al, J. Am. Chem. Soc.*, 1960, **82**, 4458.

IC-004095

$C_4H_8OReS_4^{\ominus}$

Bis(1,2-ethanedithiolato-*S,S'*)oxorhenate(*V*)(1−), 10Cl



X = O

M 386.5 (ion)
Square pyramidal, Re—S 231, Re=O 174.2 pm.

Ph_4P salt: [84825-84-3].
Synth. from K_2ReCl_5 or $ReOCl_3(PPh_3)_2$ and $HSCH_2CH_2SH$ in MeOH in presence of Et_3N, followed by addition of Ph_4PCl. Brown cryst.

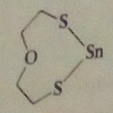
Davison, A. *et al, Inorg. Chem.*, 1980, **19**, 1988 (*synth, props*)
Blower, P.J. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 1339 (*synth, ir, pmr, cryst struct*)

$C_4H_8OS_2Sn$ IC-004096

(3-Oxapentane-1,5-dithiolato)tin

[[2,2'-Oxybis(ethanethiolato)](2−)-O,S,S']tin, 11CI

[88055-90-7]



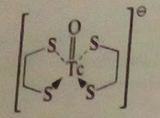
M 254.9

Pale yellow cryst. Sol. toluene. Mp 165° dec.

Tzschach, A. *et al, Z. Anorg. Allg. Chem.*, 1983, **502**, 158 (*synth*)

$C_4H_8OS_4Tc^{\ominus}$ IC-004097

Bis[1,2-ethanedithiolato(2−)-*S,S'*]oxotechnetate(*V*)(1−), 11CI, 10CI



M 299.2 (ion)

Square pyramidal anion. 1,3- and 2,3-dimercaptopropanol give analogous complexes. Synth. from $TcO_4^{\ominus}$ by $BH_4^{\ominus}$ or $S_2O_4^{2\ominus}$ redn. in presence of ligand, or from $TcOCl_4^{\ominus}$ or TcO(gluconate)$_2$ by ligand exchange. Binuclear intermediate isolated in synthesis from $TcOCl_4^{\ominus}$.

Et_4N salt: [75045-59-9].

Orange-red solid (MeOH). Mp 180-183°. Ir $\nu_{Tc=O}$ 935 cm^{-1} (KBr). Weakly paramagnetic in solid state. μ_{eff} is field strength dependent.

Ph_4As salt: [70177-06-9].

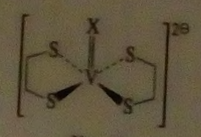
Bright orange-red cryst. (MeOH or aq. Me_2CO). Sol. Me_2CO, $CHCl_3$, MeCN; spar. sol. MeOH, EtOH; insol. H_2O, Et_2O. Mp 233-235°.

[69216-12-2]

Smith, J.E., *J. Am. Chem. Soc.*, 1978, **100**, 5571 (*synth, cryst struct*)
Byrne, E.F. *et al, Inorg. Chem.*, 1979, **18**, 1832 (*synth, uv, ir, props, pmr, cmr, powder struct*)
Jones, A.G. *et al, J. Nucl. Med.*, 1979, **20**, 641 (*synth*)
Davison, A. *et al, Inorg. Chem.*, 1980, **19**, 1988 (*synth, uv, ir, magnetism, electrochem*)
Spies, H. *et al, Inorg. Chim. Acta*, 1981, **48**, 255 (*synth, uv, ir, pmr*)
DeGregori, I. *et al, Appl. Radiat. Isot.*, 1989, **40**, 385 (*analogues*)

$C_4H_8OS_4V^{2\ominus}$ IC-004098

Bis[1,2-ethanedithiolato(2−)-*S,S'*]oxovanadate(*IV*)(2−), 11CI



X = O

M 251.3 (ion)

Square pyramidal. Various analogues are known. See also Bis[1,2-ethanedithiolato(2−)-*S,S'*]thioxovanadate(*IV*)(2−), IC-004106.

Na, Me_4N salt: [89061-84-7].

Synth. like the Na, Ph_4P salt, using $[Me_4N]Cl$. Green solid + 2EtOH (DMF/MeCN).

Na, Ph_4P salt: [97689-51-5].

Synth. from $VO(acac)_2$ and $NaSCH_2CH_2SNa$ in EtOH and adding $[Ph_4P]Br$. Green solid + 2EtOH (EtOH/Et_2O).

Di-Na salt, octa-MeOH complex: [92315-39-4]. μ_3-*Oxobis(ethane-1,2-dithiolato)vanadium*(IV)*bis*(μ-*methanol*) *hexamethanoldisodium*

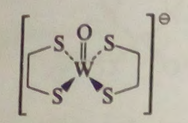
$C_{12}H_{40}Na_2O_9S_4V$ M 553.6

Synth. from Na_3VS_4 with the thiol in MeOH. Green cryst. Two Na ions are bound to oxygen of V=O, but struct. of VOS_4 unit essentially similar to that in other salts.

Wiggins, R.W. *et al, J. Chem. Soc., Chem. Commun.*, 1983, 1313 (*synth, cryst struct, mixed salt*)
Szeymies, D. *et al, Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 804 (*synth, cryst struct, di-Na salt*)
Money, J.K. *et al, Inorg. Chem.*, 1985, **24**, 3297 (*synth, cryst struct, mixed salts, ir, uv-vis, electrochem*)

$C_4H_8OS_4W^{\ominus}$ IC-004099

Bis[1,2-ethanedithiolato(2−)-*S,S'*]oxotungstate(*V*)(1−), 11CI



M 384.2 (ion)

Isomorphous with Mo analogue; W—O 164.1, W—S 236.3pm.

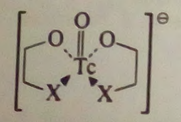
Ph_4P salt: [106608-70-2].

Obt. by thiol exchange between $[WO(SPh)_4]^{\ominus}$ and $HSCH_2CH_2SH$. Black cryst. (CH_2Cl_2/Et_2O).

Ellis, S.R. *et al, J. Chem. Soc., Chem. Commun.*, 1986, 1483 (*synth, cryst struct, esr*)

$C_4H_8O_3S_2Tc^{\ominus}$ IC-004100

Bis[2-mercaptoethanolato(2−)-*O,S*]oxotechnetate(*V*)(1−), 11CI



X = S

M 267.1 (ion)

Square-pyramidal anion. Can be reduced to Tc(*IV*) species. Synth. by dithionite redn. of $TcO_4^{\ominus}$ in presence of 2-mercaptoethanol.

Ph_4As salt: [86119-94-0].

Pink solid (Et_2O/MeCN). Sol. EtOH, MeCN; insol. Et_2O.

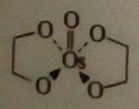
Jones, A.G. *et al, Inorg. Chem.*, 1981, **20**, 1617 (*synth, cryst struct*)
DePamphilis, B.V. *et al, Inorg. Chem.*, 1983, **22**, 2292 (*props*)
Grases, F. *et al, Bull. Soc. Chim. Fr.*, 1987, 244 (*synth, electrochem*)

$C_4H_8O_5Os$ IC-004101

Bis[ethane-1,2-diolato(2−)-*O,O'*]oxoosmium(*VI*), 9CI

Oxobis(ethane-1,2-diolato)osmium(VI)

[54260-55-8]



M 326.3

Synth. from OsO_4 + ethane-1,2-diol. Black cryst. Ir ν_{C-O} 1016s; $\nu_{Os=O}$ 992s; ν_{C-C} 868s; $\nu_{Os-Oester}$ 622m cm^{-1}.

Collin, R.J. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1094 (*synth, ir*)
Phillips, F.L. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 1814 (*cryst struct*)

$C_4H_8O_5Tc^{\ominus}$ IC-004102

Bis[1,2-ethanediolato(2−)-*O,O'*]oxotechnetate(*V*)(1−), 11CI

Oxobis(1,2-ethanediolato)technetate(V)

[91443-59-3]

As Bis[2-mercaptoethanolato(2−)-*O,S*]oxotechnetate(*V*)(1−), IC-004100 with

X = O

M 235.0 (ion)

Square-pyramidal anion. Synth. from $TcOCl_4^{\ominus}$. Starting material for synth. of dinuclear oxo-bridged aminocarboxylate species, and of bis(dithiolato) oxotechnetate complexes. Stable in (deoxygenated) H_2O at pH 10; disproportionates at pH 8.

Na salt: [86119-90-6].

Deep purple solid (EtOH).

Tetrabutylammonium salt: [111319-44-9].

Purple solid. V. sol. H_2O, polar org. solvs., C_6H_6; spar. sol. toluene; insol. Et_2O, hexane.

[97057-22-2]

DePamphilis, B.V. *et al, Inorg. Chem.*, 1983, **22**, 2292 (*reactions*)
Brenner, D. *et al, Inorg. Chem.*, 1984, **23**, 3793 (*synth, props*)
Davison, A. *et al, Inorg. Chim. Acta*, 1987, **128**, 161 (*synth, ms, uv*)
Huber, G. *et al, Polyhedron*, 1987, **6**, 1707 (*synth, ir, pmr, cmr*)
Linder, K.E. *et al, Inorg. Chem.*, 1989, **28**, 3820 (*props*)

$C_4H_8O_6Zr$ IC-004103

Bis(acetato-*O*)dihydroxyzirconium(*IV*), 11CI

Zirconium acetate hydroxide ($Zr(OAc)_2(OH)_2$). *Zirconium diacetate dihydroxide*

[14311-93-4]

$Zr(OH)_2(OAc)_2$

M 243.3

Although widely used, no synth. has been described. Commercially available. Many uses ranging from a Fischer-Tropsch catalyst, humidity sensor, concrete and fabric waterproofer, in treatment of acrylonitrile fibres, as algicide etc. White solid.

Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **20**, 72; **24**, 878 (*uses*)
Knifton, J.F. *et al, Organometallics*, 1984, **3**, 62 (*use, catalysis*)

$C_4H_8ReS_5^{\ominus}$ IC-004104

Bis(1,2-ethanedithiolato)sulfidorhenate(*V*)(1−)

Bis(1,2-ethanedithiolato-S,S')thioxorhenate(V)(*1−*), *11CI*

As Bis(1,2-ethanedithiolato-*S,S'*)oxorhenate(*V*)(1−), IC-004095 with

X = S

M 402.6 (ion)

Square pyramidal with Re—S (basal) 230, Re—S (ap.) 234 pm.

Me_4N salt: [84822-11-7].

Synth. from K_2ReCl_6 and excess of 1,2-ethanedithiol and Et_3N in MeOH, followed by addition of NMe_4Cl. Brown cryst. Ir $\nu_{Re=S}$ 517 cm^{-1}.

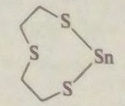
Davison, A. *et al, Inorg. Chem.*, 1980, **19**, 1988 (*synth, props*)
Blower, P.J. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 1339 (*synth, ir, pmr, cryst struct*)

$C_4H_8S_3Sn$ IC-004105

(3-Thiapentane-1,5-dithiolato)tin

[[2,2'-Thiobis(ethanethiolato)](2−)-S,S',S"]tin, 11CI

[53189-29-0]



M 271.0

Pale yellow cryst. Sol. toluene. Dec. at 144°.

Tzschach, A. *et al, Z. Anorg. Allg. Chem.*, 1983, **502**, 158 (*synth*)

$C_4H_8S_5V^{2\ominus}$ IC-004106

Bis[1,2-ethanedithiolato(2−)-*S,S'*]thioxovanadate(*IV*)(2−), 11CI

Thiobis(ethane-1,2-dithiolato)vanadate(IV)(*2−*)

As Bis[1,2-ethanedithiolato(2−)-*S,S'*]oxovanadate(*IV*)(2−), IC-004098 with

X = S

M 267.3 (ion)

Square pyramidal.

Na, Ph_4P salt: [97689-53-7].

Synth. from Bis[1,2-ethanedithiolato(2−)-*S,S'*]oxovanadate(*IV*)(2−), IC-004098 with $(Me_3Si)_2S$ in MeCN. Brown cryst. + variable Et_2O ($MeCN/Et_2O$).

Bis-Ph_4P salt: [92315-37-2].

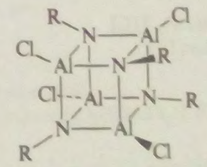
Cryst. + 1MeOH.

Szeymies, D. *et al, Angew. Chem.*, 1984, **96**, 797 (*synth, cryst struct*)
Money, J.K. *et al, Inorg. Chem.*, 1985, **24**, 3297 (*synth, cryst struct, ir*)

C_4H_9AlClN IC-004107

(*tert*-Butylimido)chloroaluminium

Chloro[2-methyl-2-propanaminato(2−)]aluminium. tert-*Butyliminochloroalane*



tetramer

R = $C(CH_3)_3$

M 133.5

Tetrameric. Bromo deriv. also descr.

Tetramer: [59236-77-0]. *Tetrachlorotetrakis[μ_3-[2-methyl-2-propanaminato(2−)]]tetraaluminium*

$C_{16}H_{36}Al_4Cl_4N_4$ M 534.2

Obt. by thermal dec. of ($^tBuNHAlHCl$)$_2$. White moisture-sensitive cryst. (by subl.). Mp 270°. Subl.$_{0.001}$ 150°.

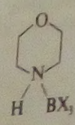
Nöth, H. *et al, Z. Naturforsch., B*, 1976, **31**, 697, 1201 (*synth, pmr, Al-27 nmr, ms*)

$C_4H_9BF_3NO$ IC-004108

Trifluoro(morpholine-N^4)boron, 10CI

Trifluoroborane morpholine. Morpholine, compd. with trifluoroborane(1:1), 9CI

[660-92-4]



X = F

M 154.9

Pisarev, M.A. *et al*, *CA*, 1973, **79**, 89955s.
Kugai, N. *et al*, *Adv. Exp. Med. Biol.*, 1977, **103**, 537.
Syutkin, E.A. *et al*, *Probl. Endokrinol.*, 1980, **26**, 53.

$C_4H_9CdClN_2O_4$ IC-004109

Aquachloro(*N*-glycylglycinato-N^N,O^O)cadmium

[50989-17-8]

$Cd(OH_2)Cl[H_2NCH_2CONHCH_2COO]$

M 296.9

Polymeric struct. with 6-coord. Cd. Synth. from $CdCl_2$ + glycylglycine at pH8. Cryst. (H_2O).

Flook, R.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 753 (*synth, cryst struct*)

$C_4H_9Cl_2OPPt$ IC-004110

Carbonyldichloro(trimethylphosphine)platinum, 10CI

Dichloro(trimethylphosphine)platinum carbonyl

M 370.0

***cis*-form** [66219-24-7]

Cryst. (CH_2Cl_2/Et_2O). Mp 196-198°.

Browning, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, raman, nmr*)

$C_4H_9Cl_2OTi$ IC-004111

Butoxydichlorotitanium(*III*), 11CI

Butanolatodichlorotitanium(III)

[32448-92-3]

$TiCl_2(OCH_2CH_2CH_2CH_3)$

M 191.9

Synth. by reaction of $TiCl_2(OBu)$ with Et_2AlCl or from $TiCl_2(OBu)_2$ with $EtAlCl_2$ in hexane. Catalyst for ethylene polym.

U.K. Pat., 1 237 169, (1969); *CA*, **75**, 110730u (*synth, use*)
Japan. Pat., 59 164 309, (1984); *CA*, **102**, 46427x (*use*)
Hu, Y. *et al*, *Gaofenzi Tongxun*, 1985, 1, 54; *CA*, **103**, 114961q (*synth, use*)

$C_4H_9Cl_2O_2V$ IC-004112

Butoxydichlorooxovanadium(*V*), 11CI

[19120-66-2]

$VOCl_2(OCH_2CH_2CH_2CH_3)$

M 210.9

Tetrahedral. Although the subject of many patents there is no synthesis in the scientific literature after 1936. Synth. from $VOCl_3$ and $Bu_3Si(OBu)$ in the presence of an amine. Olefin polym. catalyst.

Japan. Pat., 59 58 013, (1984); *CA*, **101**, 91642d (*use*)
Ger. Pat., 3 447 290, (1986); *CA*, **105**, 227023v (*synth*)

$C_4H_9Cl_3OTi$ IC-004113

Butoxytrichlorotitanium(*IV*), 11CI

Butanolatotrichlorotitanium(IV). *Titanium*(IV) *butoxide trichloride*

[3112-68-3]

$TiCl_3(OCH_2CH_2CH_2CH_3)$

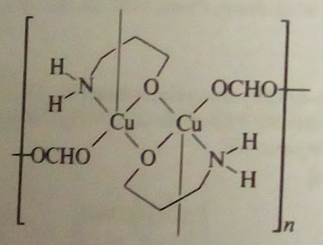
M 227.3

Synth. by reaction of $TiCl_4$ and butanol at 0°. An alternative reaction of $Ti(OBu)_4$ with MeP(O)(OPh)Cl yields $TiCl_3(OBu)$ and MeP(O)(OBu)(OPh) or from $TiCl_4$ and$(BuO)SiR_3$. It may be even be made from $Ti(OBu)_4$ + $SOCl_2$. Used extensively in Ziegler-Natta catalysts. Pale yellow solid.

Sigwalt, P. *et al*, *Bull. Soc. Chim. Fr.*, 1964, 482 (*synth, use*)
Gopinathan, C. *et al*, *Indian J. Chem.*, 1965, **3**, 136 (*synth, from $Ti(BuO)_4$ + $SOCl_2$*)
Zhinkina, L.N. *et al*, *Plast. Massy*, 1966, 23; *CA*, **65**, 18702f (*synth from $Ti(OBu)_4$*)
Sehra, J.C. *et al*, *Makromol. Chem.*, 1984, **189**, 1117 (*use*)
Czaja, K. *et al*, *Polimery (Warsaw)*, 1984, **29**, 411 (*use*)
Ger. Pat., 3 447 297, (1986); *CA*, **105**, 175282g (*synth, use*)

$C_4H_9CuNO_3$ IC-004114

(3-Aminopropanolato)formatocopper(*II*)



dimeric unit

M 182.6

Dimeric with axial formates coordinated to adjacent dimeric units.

Dimer: [112784-80-2]. *Bis[μ-(3-amino-1-propanolato*-N,O:O)*]bis(formato*-O)*dicopper*
$C_8H_{18}Cu_2N_2O_6$ M 365.3
Blue cryst. (EtOH). Insol. Me_2CO.

Sillanpää, R. *et al*, *Inorg. Chim. Acta*, 1987, **134**, 233.

$C_4H_9F_3O_3SSi$ IC-004115

Trimethylsilyl trifluoromethanesulfonate

Trimethylsilyl triflate

[27607-77-8]

$F_3CSO_2OSiMe_3$

M 222.2

Silylation reagent, catalyst for transnucleosidations. Bp_{750} 140°, Bp_{10} 36.5°.

Schmiesser, M. *et al*, *Chem. Ber.*, 1970, **103**, 868 (*synth*)
Azuma, T. *et al*, *Chem. Pharm. Bull.*, 1977, **25**, 3347.
Ende, H. *et al*, *Synthesis*, 1977, 636, 867 (*synth, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 514 (*use*)

Noyori, R. *et al*, *Tetrahedron*, 1981, **37**, 3899 (*rev*)
Demuth, M. *et al*, *Synthesis*, 1982, 827 (*synth, pmr, ms*)
Aizpurua, J.M. *et al*, *Tetrahedron Lett.*, 1985, **26**, 6113 (*pmr, synth*)

$C_4H_9FeN_2O_6P$ IC-004116

Carbonyldinitrosyl(trimethyl phosphite-*P*)iron

Carbonyldinitrosyl(phosphorous acid)iron trimethyl ester, 8CI

[21494-31-5]

$(MeO)_3PFe(NO)_2CO$

M 267.9

No phys. props. recorded.

DiStefano, G. *et al*, *J. Organomet. Chem.*, 1967, **7**, 473; 1968, **14**, 165, 465 (*synth, ms*)
Innorta, G. *et al*, *Int. J. Mass Spectrom. Ion Phys.*, 1968, **1**, 435.

$C_4H_9HgS^{\oplus}$ IC-004117

(1-Butanethiolato)mercury(1+)

Butylthiomercury(1+)

$[H_3CCH_2CH_2CH_2SHg]^{\oplus}$

M 289.7 (ion)

Prepd. in Py; monomeric when dilute; dimerises in more conc. soln. $[C_4H_9SHgHgSC_4H_9]^{2\oplus}$. Hg—Hg 369.5 pm; Py probably coord. in soln.

Perchlorate: [109710-17-0].
Synth. from $Hg(SCH_2CH_2CH_2CH_3)_2$ and $Hg(ClO_4)_2$ in Py at 60°. Not isol.

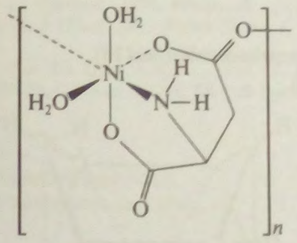
Persson, I. *et al*, *Inorg. Chim. Acta*, 1987, **129**, 47 (*synth, soln struct*)

$C_4H_9NNiO_6$ IC-004118

[2-Aminobutanedioato(2–)-*N*,*O*,*O*′]diaquanickel(*II*)

Diaqua(aspartato)nickel(II). *Aspartatodiaquanickel*(II)

[60734-59-0]



M 225.8

Polymeric chain struct. Ni octahedrally coord. Turquoise cryst. + H_2O (MeOH aq.). Sol. H_2O. Mp 207-212° dec. μ_{eff} = 3.16μ_B.

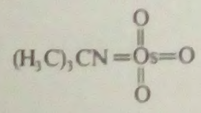
Antolini, L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 2541 (*synth, cryst struct, uv-vis, magnetism*)

$C_4H_9NO_3Os$ IC-004119

Trioxo(*tert*-butylimido)osmium

[2-Methyl-2-propanaminato(2-)]trioxoosmium, 9CI.
Trioxo(tert-*butylnitrido)osmium*. N-tert-*Butyl osmiamate*

[50381-48-1]



M 309.3

Molecular with approx. C_{3v} symmetry. Synth. from OsO_4 and $(CH_3)_3CNH_2$ in pentane chilled in a salt-ice bath. Reacts with a variety of alkenes to give, after reductive cleavage of the intermed. osmate esters, vicinal amino alcohols. Bright-yellow needles (pentane at –10°). Mp 112° dec. Subl. 40-50° *in vacuo*. Ir $\nu_{Os=N}$ 1184; $\nu_{Os=O}$ 912, 925 cm^{-1}.

Milas, N.A. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 6089 (*synth*)
Inorg. Synth., 1960, **6**, 204 (*synth*)
Miskowski, V. *et al*, *Mol. Phys.*, 1974, **28**, 747 (*uv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 641 (*use*)
Chong, A.O. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 3420 (*synth, use*)
Patrick, D.W. *et al*, *J. Org. Chem.*, 1978, **43**, 2628 (*synth, use*)
Hentges, S.G. *et al*, *J. Org. Chem.*, 1980, **45**, 2257 (*use*)

$C_4H_9NO_6PZn^{\ominus}$ IC-004120

(Acetato-*O*)[mono(2-aminoethyl)phosphato(2–)-*O*′]zincate(1–)

$[Zn(OAc)[P(O)_3OCH_2CH_2NH_2]]^{\ominus}$

M 263.4 (ion)

Phosphate groups form layers with tetrahedral zinc undulating perpendicular to the layer direction. Amino groups H-bonded to acetate groups.

H compd.: [120313-06-6].
$C_4H_{10}NO_6PZn$ M 264.4
Colourless cryst. (H_2O).

Ortiz-Avila, Y. *et al*, *Inorg. Chem.*, 1989, **28**, 2137 (*synth, cryst struct*)

$C_4H_9O_4Re$ IC-004121

(*tert*-Butanolato)trioxorhenium(*VII*)

(2-Methyl-2-propanolato)trioxorhenium(VII), *11CI.* tert-*Butyl perrhenate*

[39705-63-0]

$(H_3C)_3COReO_3$

M 307.3

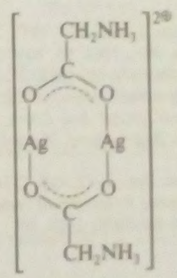
Presumed monomeric. Synth. from ReO_3Cl and $Me_3SiOC(CH_3)_3$. Colourless needles, thermally unstable at r.t. V. sol. ethers, aliphatic, aromatic and chlorinated hydrocarbons.

Edwards, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 2695 (*synth, ir, nmr, props*)

$C_4H_{10}Ag_2N_2O_4^{2\oplus}$ IC-004122

Bis(μ-glycine)disilver(2+)

(Glycine)silver(I)(*1+*) *dimer*



M 365.8 (ion)

Dinitrate: [30051-67-3].
Light-sensitive colourless cryst. Ferroelectric below –55°.

$C_4H_{10}Ag_2N_2S^{\oplus} - C_4H_{10}B_6$

Rao, J.K.M. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 1484 (*cryst struct, synth*)
Guha, S., *Indian J. Phys.*, 1932, **40**, 233 (*cryst struct*)
Pepinsky, R. *et al*, *Phys. Rev.*, 1937, **105**, 1538 (*electrical prop*)
Warrier, A.V.R. *et al*, *Proc. - Indian Acad. Sci., Sect. A*, 1967, **66**, 40 (*cr*)
Easwaran, K.R.K., *J. Phys. Soc. Jpn.*, 1965, **21**, 1614 (*pmr*)

IC-004123

$C_4H_{10}Ag_2N_2S^{\oplus}$

μ_3-[Diethylsulfonediiminato(2−)]trisilver(1+)

[μ_3-[2,2′-Sulfonimidoylbis[ethanaminato]](2−)]trisilver(1+), 9CI

[53203-30-8]

$[Ag_3(N_2SEt_2)]^{\oplus}$

M 441.8 (ion)
Struct. comprises SAg_3N tetrahedra with central N atoms linked to form double-layers.
Nitrate: Synth. from aq. $Et_2Si{=}NH)_2$ and $AgNO_3$. Similar complexes obt. for other anions.

Hass, D. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 1361 (*synth, cryst struct*)

IC-004124

$C_4H_{10}BBr$

Bromodiethylborane, 10Cl, 9Cl, 8Cl

Bromodiethylborine. Diethylbromoborane

[19162-10-8]

Et_2BBr

M 148.8
Air- and moisture-sensitive. Sol. THF.

Wiberg, E. *et al*, *Z. Anorg. Allg. Chem.*, 1933, **213**, 77 (*synth*)
Nöth, H. *et al*, *J. Organomet. Chem.*, 1968, **12**, 23 (*pmr*)
Köster, R. *et al*, *Justus Liebigs Ann. Chem.*, 1969, **719**, 169 (*synth*)
Nöth, H. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1971, 1197 (*synth*)
Haubold, W. *et al*, *Z. Anorg. Allg. Chem.*, 1976, **420**, 251 (*synth, ir*)
Paetzold, P. *et al*, *Chem. Ber.*, 1979, **112**, 663.

IC-004125

$C_4H_{10}BCl$

Chlorodiethylborane, 10Cl, 9Cl

Chlorodiethylborine. Diethylchloroborane

[5314-83-0]

Et_2BCl

M 104.3
Catalyst for polym. of alkenes and butadiene oligomerisation. Liq., sensitive to air and moisture. Bp_{100} 25°.

Buls, V.W. *et al*, *J. Am. Chem. Soc.*, 1957, **79**, 337 (*synth*)
Nöth, H. *et al*, *Chem. Ber.*, 1966, **99**, 1049 (*nmr*)
Gipstein, E. *et al*, *J. Org. Chem.*, 1966, **31**, 1087 (*synth*)
Nöth, H. *et al*, *J. Organomet. Chem.*, 1968, **12**, 23 (*nmr*)
Köster, R. *et al*, *Justus Liebigs Ann. Chem.*, 1969, **719**, 187 (*props*)
Nöth, H. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 197 (*synth*)
Barlos, K. *et al*, *Chem. Ber.*, 1977, **110**, 2774 (*nmr*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 801.

IC-004126

$C_4H_{10}BCl_2N$

Dichloro(diethylamino)borane, 8CI

1,1-Dichloro-N,N-diethylboranamine, 10CI, 9CI. Dichloro(diethylamino)borine. Diethylaminodichloroborane

[868-30-4]

Cl_2BNEt_2

M 153.8
Moisture-sensitive liq. Bp 140-146°, Bp_{20} 51-52°.
Tris-Py complex: [15590-32-6].
$C_{19}H_{20}BCl_2N_4$ M 391.1
White cryst. solid. Mp 82-86°. Hydrolyses readily in atm.

Lappert, M.F. *et al*, *J. Chem. Soc. A*, 1967, 602 (*synth*)
Greenwood, N.N. *et al*, *J. Chem. Soc. A*, 1967, 959 (*ir, synth*)
Beck, W. *et al*, *Chem. Ber.*, 1972, **105**, 2883 (*nmr*)
Lochmueller, C.H. *et al*, *J. Chromatogr.*, 1973, **85**, 132 (*chromatog*)
Nöth, H. *et al*, *Chem. Ber.*, 1981, **114**, 1150 (*cmr, nmr*)
Baudler, M. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **474**, 18 (*synth*)

IC-004127

$C_4H_{10}BCl_3O$

Trichloro(diethyl ether)boron

Trichloro[1,1′-oxybis[ethane]]boron, 10CI. Ethyl ether compd. with boron chloride (BCl_3) (1:1), 8CI. Boron trichloride etherate. Trichloroborane diethyl ether

[2102-03-6]

$Et_2O{-}BCl_3$

M 191.2
Used in catalysts for manuf. of butadiene copolymer. Moisture-sensitive.

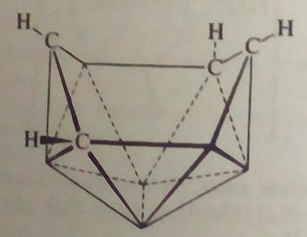
Schuster, R.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 1038 (*pmr*)
Fratiello, A. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 1194 (*nmr*)
Ger. Pat., 2 023 405, (1970); *CA*, **74**, 54901r (*use*)
Smith, J.A. *et al*, *J. Chem. Soc. A*, 1971, 178 (*nqr*)
U.S.S.R. Pat., 621 802, (1978); *CA*, **90**, 42899p.
Hu, M.G. *et al*, *Inorg. Chem.*, 1979, **18**, 3297.

IC-004128

$C_4H_{10}B_6$

5,6,8,9-Tetracarbadecaborane(10)

[120474-35-3]



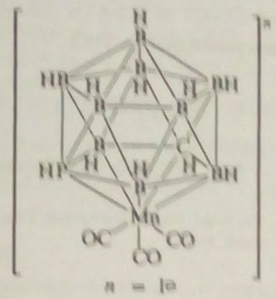
M 122.9
Synth. from *arachno*-4,5-$C_2B_7H_{13}$ with acetylene in hexane at 120° for 8 h. White cryst. (by subl.).

Hermanek, S. *et al*, *Polyhedron*, 1988, **7**, 669 (*synth*)

IC-004129

$C_4H_{10}B_6MnO_3P^{\ominus}$

Tricarbonyl[undecahydro-κ-7-phospha-9-carbaundecaborato(2−)]manganate(1−)



$n = 1^{\ominus}$

M 289.3 (ion)
7-Phenylphospha analogue also known.
Me_4N salt:
$C_8H_{22}B_6MnNO_3P$ M 363.4
Light-yellow cryst. (CH_2Cl_2/hexane). Ir ν_{CO} 2025, 1955 cm^{-1} (MeCN).

Little, J.L. *et al*, *Inorg. Chem.*, 1970, **9**, 63 (*synth, ir, uv, pmr*)

IC-004130

$C_4H_{10}BrO_3P$

Diethyl phosphorobromidate, 9CI, 8CI

Diethyl phosphoryl bromide. Diethyl bromophosphate. Diethyl bromophosphonate. Bromodiethoxooxophosphorus(V)

[51761-27-4]

$(EtO)_2P(O)Br$

M 216.9
Reagent for use in the synth. of amides and peptides in high yield with only slight racemisation. Pungent liq. $Bp_{1.5}$ 75°. n_D^{20} 1.4406, 1.4319.

Goldwhite, H. *et al*, *J. Chem. Soc.*, 1955, 3564 (*synth*)
Górecka, A. *et al*, *Synthesis*, 1978, 474 (*synth, use, ir, pmr, nmr*)
Michalski, J. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1980, 833 (*P-31 nmr*)
Kutyrev, A.A. *et al*, *Zh. Obshch. Khim.*, 1988, **58**, 484; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1988, **58**, 420 (*synth*)

IC-004131

$C_4H_{10}Br_2FeN_2S_2$

Dibromobis(thioacetamide)iron

Dibromobis(ethanethioamide-S)iron, 9CI

[19615-66-8]

$FeBr_2[S{=}C(NH_2)CH_3]_2$

M 365.9
Tetrahedral at Fe. Synth. from $FeBr_2$ in Me_2CO + Fe(powder) + $MeC(S)NH_2$. Cream cryst. ($Me_2CO/CHCl_3$). Sol. Me_2CO.

Flint, C.D. *et al*, *J. Chem. Soc. A*, 1968, 750 (*synth, ir, uv*)
Birchall, T. *et al*, *Can. J. Chem.*, 1972, **50**, 211 (*ir, mössbauer*)

IC-004132

$C_4H_{10}CdO_2$

Cadmium ethoxide ($Cd(OEt)_2$)

Diethoxycadmium. Ethanol cadmium(2+) salt (2:1)

[6982-96-3]

$Cd(OEt)_2$

M 202.5
CdI_2-type struct. Synth. from $Cd(OH)_2$ and EtOH. Catalyst for polym. of epoxides. White hygroscopic microcryst. Insol. EtOH, C_6H_6, THF. Dec. at 120°.

Turevskaya, E.P. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1968, 1377 (*synth*)
Turova, N.Ya. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1968, 2590 (*synth, ir, powder struct*)
Janekovic, A. *et al*, *Croat. Chim. Acta*, 1988, **61**, 1 (*synth, powder struct, ir, thermal anal*)

IC-004133

$C_4H_{10}ClO_3P$

Diethyl phosphorochloridite, 9CI, 8CI

Diethyl chlorophosphite. Chloro(diethoxy)phosphorus(III)

[589-57-1]

$(EtO)_2PCl$

M 156.5
Rgt. for peptide synthesis. Fuming pungent liq. d_4^{20} 1.075. Bp 153-155°, Bp_{50} 63-65°, Bp_{13} 45-50°. n_D^{20} 1.4360.
▷ Reacts explosively with H_2O.

Young, R.W. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 2126 (*synth, use*)
Michalski, J. *et al*, *J. Chem. Soc.*, 1961, 4904 (*synth*)
Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **307**, 113 (*P-31 nmr*)
Jones, R.A.Y. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1962, **1**, 32 (*nmr*)
Gloede, J. *et al*, *J. Prakt. Chem.*, 1974, **316**, 703 (*synth, nmr*)
Malenko, D.M. *et al*, *Zh. Obshch. Khim.*, 1979, **49**, 308; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1979, **49**, 267 (*synth, P-31 nmr*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 672.

IC-004134

$C_4H_{10}ClO_3Sb$

Chlorodiethoxystibine, 8CI

Chlorodiethoxoantimony

[59717-80-5]

$(EtO)_2SbCl$

M 247.3
Needles (pet. ether). Insol. Et_2O, hexane. Mp 106-107°. Bp_{10} 120-122°.

Arbuzov, B.A. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 390; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1976, 370 (*synth, ir, raman*)
Binder, G.E. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **471**, 121; 1983, **507**, 163 (*ms, cryst struct, ir, raman*)

IC-004135

$C_4H_{10}ClO_2Ti$

Chlorodiethoxytitanium(*III*), 11Cl

[88092-84-6]

$TiCl(OEt)_2$

M 173.4
Probably polymeric. Synth. by reaction of $TiCl_3$ with excess triethyl orthoformate. Yellow-brown solid. Mp 270° dec.

Giannetti, E. *et al*, *Inorg. Chim. Acta*, 1983, **74**, 215 (*synth, ir*)

IC-004136

$C_4H_{10}ClO_3V$

Chlorodiethoxyoxovanadium(*V*), 11Cl

[1635-99-0]

$VOCl(OEt)_2$

M 192.5
Tetrahedral. Synth. either from $VOCl_3$ and NaOEt or from $VOCl_3$, $Et_2Si(OEt)_2$ and an amine. Olefin polym. catalyst.

Gervais, D. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 3679 (*synth, ir, uv, pmr*)
Rehder, D., *Z. Naturforsch., B*, 1977, **32**, 771 (*V-51 nmr*)
U.S. Pat., 4 435 518, (1984); *CA*, **100**, 175531j (*use*)
Ger. Pat., 3 447 290, (1986); *CA*, **105**, 227023v (*synth*)

IC-004137

$C_4H_{10}ClPS_2$

Diethyl phosphorochloridodithioite, 9CI

Diethyl dithiochlorophosphite. Chlorobis(ethylthio) phosphorous(III)

[1486-42-6]

$(EtS)_2PCl$

M 188.6
Liq. Bp_{10} 108°, Bp_5 84-85°, $Bp_{0.02}$ 48-50°. n_D^{20} 1.5793.

Sinyashin, O.G. *et al, Zh. Obshch. Khim.*, 1981, **51**, 2410; 1983, **53**, 502, 1706; 1985, **55**, 453; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1981, **51**, 2078; 1983, **53**, 436, 1535; 1985, **55**, 401 (*synth, P-31 nmr*)
Kostin, V.P. *et al, Zh. Obshch. Khim.*, 1982, **52**, 498; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1982, **52**, 437 (*synth*)

IC-004138

$C_4H_{10}ClPS_3$

Diethyl phosphorochloridotrithioate, 9CI, 8CI

Diethyl chlorotrithiophosphate. Chlorobis(ethylthio) thiophosphorus(V)

[16001-01-7]

$(EtS)_2P(S)Cl$

M 220.7
Liq. Bp_2 110-113°.
▷ Vesicant.

Mastin, T.W. *et al, J. Am. Chem. Soc.*, 1945, **67**, 1662 (*synth*)

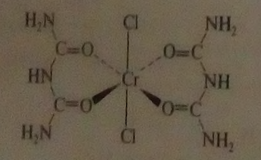
IC-004139

$C_4H_{10}Cl_2CrN_6O_4$

Dichlorobis(imidodicarbonicdiamide-*O,O'*)chromium(*II*), 10CI

Bis(biuret)dichlorobischromium(II)

[67606-96-6]



M 329.0
High spin, temp. independent μ_{eff} suggests monomeric compd. with 6-coord. Cr. Ir data indicates Cr—O coordn. Synth. from biuret + $CrCl_2.4H_2O$ in EtOH. Pale blue microcryst. μ_{eff} = 4.85μ_B (295K, 90K).

Larkworthy, L.F. *et al, Inorg. Chim. Acta*, 1978, **28**, 251 (*magnetism, ir, uv-vis, struct, synth*)

IC-004140

$C_4H_{10}Cl_2FeN_2S_2$

Dichlorobis(thioacetamide)iron(*II*)

Dichlorobis(ethanethioamide-S)iron, 9CI

[35789-49-2]

$FeCl_2[S{=}C(NH_2)CH_3]_2$

M 277.0
Tetrahedral at Fe. Synth. from $FeCl_2$ in Me_2CO or EtOH + Fe (powder) + thioacetamide. μ_{eff} = 5.27μ_B (295K).

Nardelli, M. *et al, Gazz. Chim. Ital.*, 1957, **87**, 1478 (*synth*)
Livingstone, S.L., *Q. Rev., Chem. Soc.*, 1965, **19**, 386.

Flint, C.D. *et al, J. Chem. Soc. A*, 1968, 750 (*uv, ir*)
Birchall, T. *et al, Can. J. Chem.*, 1972, **50**, 211 (*ir, synth, magnetism, mössbauer*)

IC-004141

$C_4H_{10}Cl_2HfO_2$

Dichlorodiethoxyhafnium(*IV*), 11CI

[105137-30-2]

$(EtO)_2HfCl_2$ (C_{2v})

M 339.5
May be used to form HfO_2 anti-reflective coatings on glass.

Sviridova, A.I., *Zh. Prikl. Khim.* (*Leningrad*), 1986, **59**, 1436; *CA*, **105**, 196017 (*synth, hydrol*)

IC-004142

$C_4H_{10}Cl_2HgN_6O_4$

Dichlorobis(imidodicarbonic diamide-*O*)mercury(*II*), 10CI

Bis(biuret)dichloromercury(II). *Bis(biuret)mercury dichloride*

[67489-81-0]

$[H_2NCONHC(NH_2){=}O]_2HgCl_2$

M 477.6
Struct. comprises infinite polymers, 6-coordinate Hg is linked by double O bridge to 2 Cl and four amide O. Needles (H_2O).

[12545-31-2]

Aida, K. *et al, J. Inorg. Nucl. Chem.*, 1961, **23**, 155 (*ir*)
McLellan, A.W. *et al, J. Chem. Soc. A*, 1967, 137 (*synth, ir*)
Nuttall, R.H. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 2979 (*ir*)
Saito, Y. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 2089 (*ir*)
Birker, P.J.M.W.L. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 182 (*cryst struct, ir*)
Tooru, Y. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 1561 (*pe*)
Konovalov, L. *et al, J. Coord. Chem.*, 1986, **14**, 201 (*ir*)

IC-004143

$C_4H_{10}Cl_2HgS$

Dichloro(diethyl sulfide)mercury(*II*)

Dichloro[1,1'-thiobis[ethane]]mercury(II), *10CI*

$(Et_2S)HgCl_2$

M 361.6
Polymeric in solid state. Cryst. (EtOH or Me_2CO/Et_2S). Mp 76.5-77°. Loses Et_2S on grinding crystals, to give $(Et_2S)_2(HgCl_2)_3$ and $(Et_2S)(HgCl_2)_2$. Crystallisation from Me_2CO or C_6H_6 provides $(Et_2S)(HgCl_2)_2$.

Dimer: Di-μ-chlorodichlorobis(ethyl sulfide)dimercury $C_8H_{20}Cl_4Hg_2S_2$ M 723.3

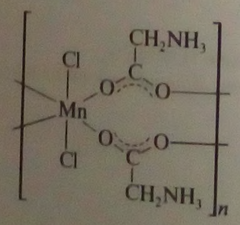
Wegscheider, R. *et al, Monatsh. Chem.*, 1919, **40**, 323 (*synth*)
Faragher, W.F. *et al, J. Am. Chem. Soc.*, 1929, **51**, 2774.
Biscarini, P. *et al, J. Chem. Soc. A*, 1969, 2206 (*synth, ir*)
Buck, K.R., *Inorg. Nucl. Chem. Lett.*, 1979, **15**, 117 (*ir*)

IC-004144

$C_4H_{10}Cl_2MnN_2O_4$

Dichlorobis(glycine)manganese(*II*), 9CI

[53846-03-0]



M 275.9
Polymeric struct. with *trans*-octahedral Mn. Synth. from aq. $MnCl_2$ and glycine in stoichiometric proportions. Dec. > 200° to Mn_2O_3. Mn migrates to cathode during electrolysis. Sol. H_2O, EtOH, Me_2CO, hot $HOCH_2CH_2OH$; sl. sol. Et_2O, $CHCl_3$, C_6H_6.

Berezina, L.P. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 1633 (*props*)
Narayanan, P. *et al, Z. Kristallogr.*, 1975, **142**, 52 (*synth, cryst struct*)
Berezina, L.P. *et al, J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 1393 (*ir, elec cond*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 256 (*rev, bibl*)

IC-004145

$C_4H_{10}Cl_2MnO_2$

Dichloro(1,2-dimethoxyethane-*O,O'*)manganese(*II*), 9CI

[25867-46-3]

$MnCl_2(MeOCH_2CH_2OMe)$

M 215.9
Synthesis of this compd. from $MnCl_2$ and $MeOCH_2CH_2OMe$ could not be repeated. Polymeric octahedral struct. proposed. Synth. by passing dry Cl_2 into a suspension of Mn powder in $MeOCH_2CH_2OMe$. White. Mp 235°.

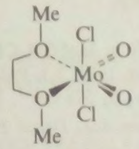
Fowles, G.W.A. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 3119 (*synth, ir, uv, magnetism*)
Hengge, E. *et al, Monatsh. Chem.*, 1972, **103**, 418 (*synth, ir, magnetism*)
Chaudhuri, N.Ray. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 2837 (*synth, therm.al dec*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 140 (*rev, bibl*)

IC-004146

$C_4H_{10}Cl_2MoO_4$

Dichloro(1,2-dimethoxyethane-*O,O'*) dioxomolybdenum(*VI*), 11CI

[84825-88-7]



M 288.9
Has distorted octahedral config. Synth. from MoO_2Cl_2 and 1,2-dimethoxyethane. White cryst.

Kamenar, B. *et al, Inorg. Chim. Acta*, 1982, **65**, L245 (*synth, cryst struct*)

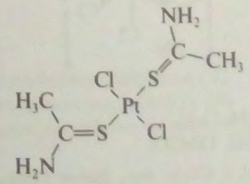
IC-004147

$C_4H_{10}Cl_2N_2PtS_2$

Dichlorobis(thioacetamide)platinum(*II*)

Dichlorobis(ethanethioamide)platinum, 9CI

[60648-84-2]



M 416.2
Unusual example of *trans*-structure for thio-ligand. Yellow solid.

Sibiriskaya, V.Y. *et al, Zh. Obshch. Khim.*, 1976, **46**, 1883.

IC-004148

$C_4H_{10}Cl_2N_2S_2Zn$

Dichlorobis(thioacetamide-S')zinc

Dichlorobis(ethanethioamide-S)zinc, 10CI. Bis(thioacetamide) zinc dichloride

[17993-05-4]

$ZnCl_2[S{=}C(CH_3)NH_2]_2$

M 286.5
Tetrahedral at Zn. Cryst.

Nardelli, M. *et al, Gazz. Chim. Ital.*, 1957, **87**, 1478 (*synth*)
Gosavi, R.K. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1937 (*synth, ir*)
Flint, C.D. *et al, J. Chem. Soc. A*, 1968, 750 (*ir*)
Rolies, M. *et al, Cryst. Struct. Commun.*, 1977, **6**, 275 (*cryst struct*)

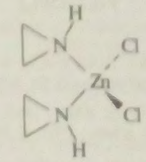
IC-004149

$C_4H_{10}Cl_2N_2Zn$

Bis(aziridine)dichlorozinc

Bis(aziridine)zinc dichloride. Zinc(II) *chloride bis(aziridine). Dichlorobis(ethylenimine)zinc*

[27184-23-2]



M 222.4
Cryst. (EtOH). Insol. Et_2O. Mp 88°.

[28475-82-3]

Nametkin, N.S., *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1972, 1874 (*synth, ir*)
Razumova, E.P. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 178 (*synth, ir, raman*)
Mirskova, I.S. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **237**, 346 (*ir, raman*)
Perchenko, V.N. *et al, Koord. Khim.*, 1985, **11**, 161 (*ir, thermal anal*)

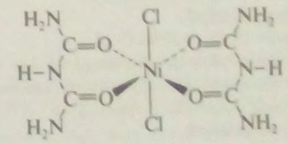
IC-004150

$C_4H_{10}Cl_2N_6NiO_4$

Dichlorobis(imidodicarbonic diamide-*O,O'*)nickel, 9CI

Bis(biuret)dichloronickel, 8CI

[25999-74-0]



M 335.7
Approx. octahedral.

trans-form [89709-40-0]
Pale green solid. Mp 302° dec.

[55467-83-9]

McLellan, A.W. *et al, J. Chem. Soc. A*, 1967, 137 (*synth, struct, ir*)
Mabiala, N. *et al, Polyhedron*, 1984, **3**, 99 (*synth, struct, ir, props*)

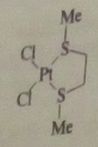
IC-004151

$C_4H_{10}Cl_2PtS_2$

Dichloro(2,5-dithiahexane)platinum(*II*)

Dichloro[1,2-bis(methylthio)ethane]platinum, 8CI

[15407-56-4]



M 388.2

Complex chiral at sulfur. Yellow solid. Sol. various org. solvs. Mp 226°.

Morgan, G.T. *et al, J. Chem. Soc.*, 1934, 965 (*synth*)
Rice, D.A. *et al, Spectrochim. Acta, Part A*, 1971, **27**, 279 (*ir*)
Hartley, F.R. *et al, Inorg. Chim. Acta*, 1979, **35**, 265 (*uv-vis, pmr*)

IC-004152

$C_4H_{10}Cl_3FeO$

Trichloro(diethyl ether)iron(*III*)

Iron(III) *chloride etherate. Ferric chloride etherate. Iron trichloride etherate*

[3928-00-5]

$FeCl_3(OEt_2)$

M 236.3

Tetrahedral at Fe. Obt. from $FeCl_3$ + Et_2O. Hydrogenation catalyst (with Et_3Al).

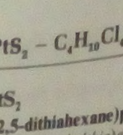
Fomin, V.V. *et al, Zh. Neorg. Khim.*, 1960, **5**, 1385 (*synth*)
Jain, S.R. *et al, Indian J. Chem.*, 1965, **3**, 223.

$C_4H_{10}Cl_3NTi$ IC-004153

***catena*-Trichloro(diethylamido)titanium(*IV*)**

Trichloro(N-ethylethanaminato)titanium(IV), *9CI*

[31885-39-9]



M 226.3

Polymer formed by octahedra sharing edges. Synth. from $TiCl_4$ and Me_3SiNEt_2 in C_6H_6 or by reaction of $Ti(NEt_2)_4$ with $TiCl_4$ in C_6H_6. Olefin polym. catalyst. Sol. C_6H_6, pet. ether. Mp 85-86°, Mp 76-78°.

Et_4NCl complex (1:1): [40956-88-5].
Olefin polym. catalyst.

Et_4NCl complex (1:2): [40956-89-6].
Pentachloro(diethylamido)titanate(2−), bis-tetraethylammonium salt. Bis(tetraethylammonium) pentachloro(diethylamido)titanate(2−)
Olefin polym. catalyst.

Japan. Pat., 665 379, (1963); *CA*, **65**, 4714a (*synth from $Ti(NEt_2)_4$*)
Burger, H. *et al, Z. Anal. Chem.*, 1969, **365**, 243 (*synth, ir, raman, pmr*)
Italian Pat., 867 243, (1970); *CA*, **79**, 19427x (*use*)
Fuyos, J. *et al, Z. Anorg. Allg. Chem.*, 1971, **380**, 196 (*cryst struct*)
Fr. Pat., 2 103 071, (1972); *CA*, **78**, 44266t (*use*)
Ger. Pat., 2 137 872, (1972); *CA*, **76**, 141538n (*use*)

$C_4H_{10}Cl_3O_2Ta$ IC-004154

Trichlorodiethoxytantalum(*V*), 11CI

[44916-29-2]

$TaCl_3(OEt)_2$

M 377.4

Synth. from $TaCl_5$ and EtOH.

EtOAc complex: [18476-50-1].
$C_8H_{18}Cl_3O_4Ta$ M 465.5
Synth. by adding AcCl to $Ta(OEt)_5$ in C_6H_6. Light brown liq.

Funk, H. *et al, Ber.*, 1929, **62**, 1688 (*synth*)
Kapoor, R.N. *et al, Indian J. Chem.*, 1967, **5**, 442 (*synth, deriv*)

$C_4H_{10}Cl_3RuS_2$ IC-004155

[1,2-Bis(methylthio)ethane]trichlororuthenium(*III*)

$[RuCl_3(MeSCH_2CH_2SMe)]_n$

M 329.6

Polymeric. Brown solid. $\mu_{eff} = 1.25\mu_B$.

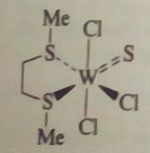
Rice, D.A. *et al, Inorg. Chim. Acta*, 1971, **5**, 683 (*synth, ir, magnetism*)

$C_4H_{10}Cl_3S_3W$ IC-004156

Trichloro(2,5-dithiahexane)sulfidotungsten(*V*)

[1,2-Bis(methylthio)ethane-S,S']trichlorothiooxotungsten(V), *10CI, 9CI*

[55907-23-8]



M 444.5

Distorted octahedral. First struct. containing a W(*V*) sulfido-halide moiety.

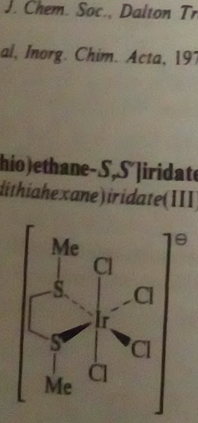
***mer*-form** [70749-27-8]
Synth. from WCl_4S + $MeSCH_2CH_2SMe$ in $CHCl_3$ for 3 weeks. Orange cryst. ($CHCl_3$). Paramagnetic, μ_{eff} = $1.45\mu_B$ (298K). Ir $\nu_{W=S}$ 528 cm^{-1}. Broad esr signal.

Britnall, D. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 213 (*synth, ir*)
Drew, M.G.B. *et al, Inorg. Chim. Acta*, 1979, **34**, L192 (*cryst struct*)

$C_4H_{10}Cl_4IrS_2^{\ominus}$ IC-004157

[1,2-Bis(methylthio)ethane-*S,S'*]iridate(1−), 10CI

Tetrachloro(2,5-dithiahexane)iridate(III)(*1−*)



M 456.2 (ion)

Me_4N salt: [75674-55-4].
Fawn solid. Sol. DMSO.

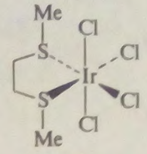
Gulliver, D.J. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1872 (*synth, ir, pmr, uv, magnetism, props*)

$C_4H_{10}Cl_4IrS_2$ IC-004158

[1,2-Bis(methylthio)ethane-*S,S'*]tetrachloroiridium(*IV*), 10CI

Tetrachloro(2,5-dithiahexane)iridium(IV)

[75674-45-2]



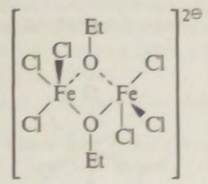
M 456.2

Red-purple solid. Sol. DMSO.

Gulliver, D.J. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1872 (*synth, ir, uv*)

$C_4H_{10}Cl_6Fe_2O_2^{\ominus}$ IC-004159

Hexachlorodi-μ-ethoxydiferrate(2−)



M 414.5 (ion)

Fe(*III*) centres are antiferromagnetically coupled.

*Bis[tri-*tert*-butylphosphonium] salt:* [125330-21-4].
*Dihydrogen salt, compd. with tri-*tert*-butylphosphine*
$C_{14}H_{33}Cl_3FeOP$ M 410.5
Synth. from $FeCl_3(P^tBu_3)$ heated under reflux in EtOH. Air stable yellow-orange cryst. (EtOH/heptane). Sol. $CHCl_3$. μ_{eff} = $4.07\mu_B$ per Fe.

Walker, J.D. *et al, Inorg. Chem.*, 1990, **29**, 757 (*synth, struct, ir, uv, magnetitism*)

$C_4H_{10}CrN_2O_5$ IC-004160

Aquabis(glycinato-*N,O*)chromium(*II*), 10CI, 8CI

Bis(glycinato)chromium(II) *monohydrate*

[62747-05-1]

$Cr(OOCCH_2NH_2)_2(OH_2)$

M 218.1

Poss. square pyramidal. Pale violet air-sensitive cryst. Insol. EtOH and other org. solvs.; sol. H_2O with dec. μ_{eff} = 4.61 (295K), $4.52\mu_B$ (90K).

[15203-46-0]

Lux, H. *et al, Chem. Ber.*, 1964, **97**, 503 (*synth, struct*)
Herzog, S. *et al, Z. Chem.*, 1966, **6**, 344.
Larkworthy, L.F. *et al, Inorg. Chim. Acta*, 1977, **21**, 265 (*synth, uv*)
Micskei, K., *J. Chem. Soc., Dalton Trans.*, 1983, 1335 (*stability const*)

$C_4H_{10}F_5NW$ IC-004161

(Diethylamido)pentafluorotungsten(*VI*)

Diethylaminopentafluorotungsten(VI). (N-*Ethylethanaminato)pentafluorotungsten*(VI), *9CI*

[30746-62-4]

Et_2NWF_5

M 350.9

Probably octahedral. Synth. from WF_6 and Me_3SiNEt_2. Moisture-sensitive viscous, dark red-brown oil.

Majid, A. *et al, Z. Anorg. Allg. Chem.*, 1971, **385**, 85 (*synth, pmr, ir, reactions*)
Majid, A. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1876 (*synth*)
Fraser, C.J.W. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 1535 (*ligand exchange*)

$C_4H_{10}FeN_2O_2S_2^{\ominus}$ IC-004162

Bis(ethanethiolato)dinitrosylferrate(1−)

[97773-70-1]

$[Fe(NO)_2(SEt)_2]^{\ominus}$ (C_{2v})

M 238.1 (ion)

Obt. from diamagnetic dimer by reaction with nucleophile. Associated with cancerous states in animals. Paramagnetic.

Butler, A.R. *et al, Polyhedron*, 1985, **4**, 797 (*synth, esr*)

$C_4H_{10}Fe_2N_4O_4S_2$ IC-004163

Bis(μ-ethanethiolato)tetranitrosyldiiron

Diethyltetranitrosyldi-μ-thioxodiiron, 10CI. Roussin's red ethyl ester, 10CI

[15020-36-7]

As Tetranitrosylbis(trifluoromethanethiolato)diiron, IC-002933 with

R = Et

M 353.9

Exists as a mixt. of *syn*- and *anti*-isomers in soln. Red-black plates (pentane); mod. air-sensitive. Mp 78.5-80°. Ir ν_{NO} 1778vs, 1750vs cm^{-1} ($CHCl_3$).

[15696-36-3, 88643-18-9, 88643-19-0]

Pavel, O., *Ber.*, 1882, **15**, 2600 (*synth*)
Hoffmann, K.A. *et al, Z. Anorg. Allg. Chem.*, 1895, **9**, 295 (*synth*)
Manchot, W. *et al, Chem. Ber.*, 1926, **59**, 412; 1927, **60**, 2318 (*ir, synth*)
Thomas, J.T. *et al, Acta Crystallogr.*, 1958, **11**, 599 (*struct*)
Wetherill, T.D. *et al, Inorg. Chem.*, 1986, **25**, 1466 (*exafs*)
Seyferth, D. *et al, Organometallics*, 1986, **5**, 539 (*synth, ir, pmr, cmr, ms*)

$C_4H_{10}HgO_2$ IC-004164

Mercury(*II*) ethoxide

Diethoxymercury(II). *Ethanol mercury(2+) salt*

[21350-48-1]

$Hg(OEt)_2$

M 290.7

Synth. from $Hg(OH)_2$ and EtOLi. Catalyst for polym. of epoxides. Thermally unstable, hygroscopic yellow solid. Insol. EtOH, C_6H_6, THF. Dec. at 127°.

Turova, N.Ya. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 2590 (*synth, ir*)
Turevskaya, E.P. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 1577 (*synth*)

$C_4H_{10}HgS_2$ IC-004165

Bis(ethylthio)mercury

Bis(ethanethiolato)mercury. Mercury ethanethiolate

[811-50-7]

EtSHgSEt

M 322.8

Monomeric in $CHCl_3$ and Py with linear Hg (v. weak additional contacts with 4 other S). Component of Ziegler catalyst combinations. Cryst. (EtOH). Sol. $CHCl_3$. Mp 72-73°.

[64762-06-7]

Landa, S. *et al*, *Collect. Czech. Chem. Commun.*, 1959, **24**, 2197 (*synth*)
Bradley, D.C. *et al*, *Can. J. Chem.*, 1965, **43**, 2786 (*cryst struct*)
Biscarini, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2140 (*synth, ir, raman*)
Canty, A.J. *et al*, *Inorg. Chim. Acta*, 1976, **20**, 161; 1977, **24**, 109 (*ir, pmr*)
Peringer, P., *Monatsh. Chem.*, 1980, **111**, 1245 (*Hg-199 nmr*)
Biscarini, P. *et al*, *Inorg. Chim. Acta*, 1981, **50**, 243 (*pe*)
Dean, P.A.W. *et al*, *Inorg. Chem.*, 1987, **26**, 4245 (*Hg-199 nmr*)

$C_4H_{10}LiN$ IC-004166

Lithium diethylamide

N-Ethylethanamine lithium salt, 9CI. N,N-*Diethylamine lithium salt, 8CI*

[816-43-3]

$LiNEt_2$

M 79.0
Commercially available. Strong base used in synth. Solid.

▷ Pyrophoric; corrosive.

Cope, A.C. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 2844.
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 331.
Xie, R. *et al*, *Huaxue Shiji*, 1982, 105; *CA*, **97**, 71588 (*rev*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2154B.

$C_4H_{10}MgO_2$ IC-004167

Magnesium ethoxide

Diethoxymagnesium. Ethanol, magnesium salt, 9CI. Ethyl alcohol, magnesium salt, 8CI

[2414-98-4]

$Mg(OEt)_2$

M 114.4
Prepd. by reaction of Mg with EtOH under strictly anhydrous conditions. Activators such as $HgCl_2$ can by used to promote reaction. Commercially available. Catalyst for polym. of olefins. Colourless moisture sensitive hexagonal cryst. Reacts with $H_2O \rightarrow$ EtOH + $Mg(OH)_2$. Calcination in air or under vacuum yields, without hydrolysis, MgO. Sol. EtOH; insol. C_6H_6; insol. THF. Mp >300°.

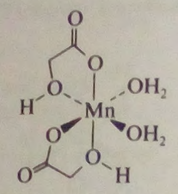
▷ Flammable.

Turova, N.Ya. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1967, **3**, 1435 (*struct*)
Lutz, H.D., *Z. Anorg. Allg. Chem.*, 1968, **356**, 132 (*ir*)
Dongare, M.K. *et al*, *Thermochim. Acta*, 1982, **57**, 37 (*dta*)
Hattori, T. *et al*, *J. Mater. Sci. Lett.*, 1983, **2**, 504 (*synth, calcination*)
Eur. Pat., 186 294, (1986); *CA*, **105**, 136473 (*synth*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2179A.

$C_4H_{10}MnO_8$ IC-004168

Diaquabis(2-hydroxyacetato-*O*,*O*˝)manganese(*II*)

Diaquabis(glycollato)manganese(II)



M 241.0
Octahedral. Synth. from $MnCO_3$ and glycollic acid. Neutral molecules are held together via hydrogen bonds.

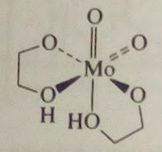
Lis, T., *Acta Crystallogr., Sect. B*, 1980, **36**, 701 (*synth, cryst struct*)

$C_4H_{10}MoO_6$ IC-004169

Bis(1,2-ethanediolato-*O*,*O*˙)dioxomolybdenum(*VI*), 11Cl, 10Cl, 9Cl

Dioxobis(2-hydroxyethanolato)molybdenum(VI)

[55397-36-9]



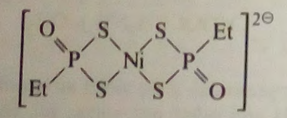
M 250.0
cis-Octahedral. Catalyses epoxidation of alkenes by hydroperoxides. Colourless cryst. (EtOH). Sol. EtOH. Ir $\nu_{Mo=O}$ 948, 920 cm^{-1}.

Schroder, F.A. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 531 (*cryst struct*)
Kesarev, S.A., *CA*, 1977, **87**, 167218k (*use*)
Knobler, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 248 (*synth, ir*)
Eur. Pat., 138 624, (1985); *CA*, **103**, 76884 (*use*)

$C_4H_{10}NiO_2P_2S_4^{2\ominus}$ IC-004170

Bis(ethylphosphonodithioato-*S*,*S*˝)nickelate(*II*)(2−), 9Cl

Bis(ethyldithiophosphonato)nickelate(II)(2−)



M 339.0 (ion)
Square planar. Rare example of phosphorodithioate containing alkyl and *O*-alkyl substituents.

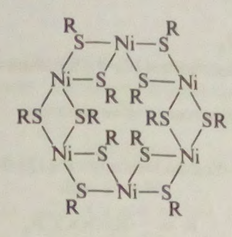
Bis-EtNH$_3$ salt: [68831-04-9]
Formed during synth. of $Ni(S_2PEt_2)_2$. Purple needles.

Arora, S.K. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3355 (*cryst struct*)

$C_4H_{10}NiS_2$ IC-004171

Bis(ethanethiolato)nickel(*II*)

Bis(ethylthio)nickel(II). *Bis(ethylmercapto)nickel*(II). *Nickel*(II) *ethylmercaptide*



hexamer
R = Et

M 180.9
Hexameric crown-like struct. Also obtd. as higher molecular mass polymer which is insol. C_6H_6.

Hexamer: Dodecakis[μ-(*ethanethiodato*)]*hexanickel*(II)
$C_{24}H_{60}Ni_6S_{12}$ M 1085.6
Purple-black or dark brown cryst. (Me_2CO/CH_2Cl_2 or hexane). Sol. C_6H_6, hexane.

Woodward, P. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 5251 (*cryst struct*)
Bladon, P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1965, 557 (*synth*)
Abel, E.W. *et al*, *J. Chem. Soc. A*, 1966, 1377 (*synth*)

$C_4H_{10}OZn$ IC-004172

(*tert*-Butoxy)(hydrido)zinc

$HZnOC(CH_3)_3$

M 139.5
Tetrameric in gas phase.

Tetramer: [119656-28-9]. *Tetrakis(2,2-dimethylpropyloxy) tetrahydrotetrazinc*
$C_{16}H_{40}O_4Zn_4$ M 558.0
Cryst. Mp 165-167° dec.

Neils, T.L. *et al*, *Inorg. Chem.*, 1989, **28**, 1607 (*synth, pmr, ir, ms*)

$C_4H_{10}O_2Sn$ IC-004173

Tin(*II*) ethoxide

Diethoxytin. Ethanol, tin(2+) salt (2:1)

[14791-99-2]

$Sn(OEt)_2$

M 208.8
Synth. from $SnCl_2$ + EtOH in the presence of Et_3N. White solid.

Morrison, J.S. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 393 (*synth, ir*)
Athar, T. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1989, **19**, 195 (*ir, nmr*)

$C_4H_{10}O_2Zn$ IC-004174

Zinc ethoxide

Ethanol, zinc salt

[3851-22-7]

$Zn(OEt)_2$

M 155.5
Prepd. from $Zn(OMe)_2$ + EtOH in the presence of Li. Non-volatile white solid. Insol. EtOH.

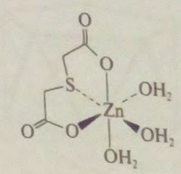
Mehrotra, R.C. *et al*, *Z. Anorg. Allg. Chem.*, 1969, **370**, 300 (*synth*)

$C_4H_{10}O_7SZn$ IC-004175

Triaqua[[2,2′-thiobis[acetato]](2−)-*O*^{1},*O*^{1}′,*S*^{2}]zinc, 9CI

Triaquazinc thiodiglycolate

[55220-02-5]



M 267.5
fac-Octahedral. Air-stable cryst. (H_2O). Forms a monohydrate.

Prochazkova, O. *et al*, *Collect. Czech. Chem. Commun.*, 1973, **38**, 1120 (*synth, ir, struct, stab const*)
Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 144 (*cryst struct*)

$C_4H_{10}O_8Pb_3$ IC-004176

Lead acetate hydroxide ($Pb_3(OAc)_2(OH)_4$)

Lead subacetate. Bis(acetato-O)tetrahydroxytrilead

[1335-32-6]

$Pb(OAc)_2.2Pb(OH)_2$

M 807.7
Synth. from conc. aq. ammonia and lead acetate in H_2O. White monoclinic or gelatinous solid. V. sol. cold H_2O.

▷ Toxic. OF8750000.

Gundurao, S.N. *et al*, *Proc. Annu. Conv. Sugar Technol. Assoc. India*, 1958, **26**, 60.
Gmelin Handbook Inorg. Chem., Syst. No. 47, 1969, **C2**, 775 (*rev, bibl*)
Chan, C.C., *Publ. Tech. Pap. Proc. Annu. Meet. Sugar Ind. Technol.*, 1987, **46**, 1.

$C_4H_{11}BO$ IC-004177

Trihydro(tetrahydrofuran)boron, 10Cl

Borane tetrahydrofuran. Tetrahydrofuran compd. with borane(1:1), 9CI, 8CI

[14044-65-6]

As Trifluoro(tetrahydrofuran)boron, IC-004056 with

X = H

M 85.9
Hydroborating and reducing agent. Produced commercially. Used only in soln., unstable in pure state, moisture-sensitive.

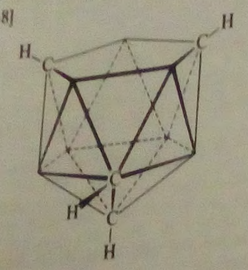
▷ Flammable.

Coyle, T.D. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 2989 (*synth*)
Fratiello, T.P.O. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 1194 (*nmr*)
Dodds, A.R. *et al*, *Inorg. Chem.*, 1977, **16**, 2900.
Compr. Org. Chem., Pergamon, Oxford, 1979, **3**, 695 (*rev*)
Nöth, H. *et al*, *Inorg. Chem.*, 1981, **20**, 1062.
Kabalka, G.W. *et al*, *J. Org. Chem.*, 1981, **46**, 4582.
Stanfield, C.F. *et al*, *J. Org. Chem.*, 1981, **46**, 4799.
Marsella, J.A. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 2361.
Paroli, R.M. *et al*, *Inorg. Chem.*, 1989, **28**, 1819 (*ir, raman*)
Fontaine, X.L.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1990, 681 (*pmr, B-11 nmr*)

$C_4H_{11}B_7$ IC-004178

1,2,8,10-Tetracarbaundecaborane(11), 11Cl

[85701-88-8]



M 134.8

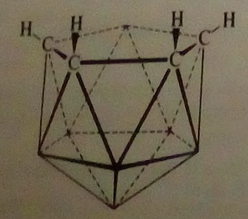
nido-. Air-stable colourless solid (by glc). Sol. $CHCl_3$. Mp 204-205° (sealed tube).

Astheimer, R.J. *et al, Inorg. Chem.*, 1983, **22**, 1928 (*synth, pmr, B-11 nmr, cmr, ir, ms, glc*)

$C_4H_{11}B_7$ IC-004179

7,8,9,10-Tetracarbaundecaborane(11)

[120396-06-7]



M 134.8

nido-. Obt. by thermal dec. of $[C_4B_7H_{12}]^{\ominus}$ at 140°.

Hermanek, S. *et al, Polyhedron*, 1988, **7**, 669 (*synth, ms, nmr*)

$C_4H_{11}B_7FeO_4$ IC-004180

Tetracarbonyl(η³-heptaborane(11))iron, 9Cl

[54190-57-7]

M 254.6

Structure unknown but see derived anion, Tetracarbonyl[η³-dodecahydroheptaborato(1−)] ferrate(1−), IC-004205. Mp ~20°.

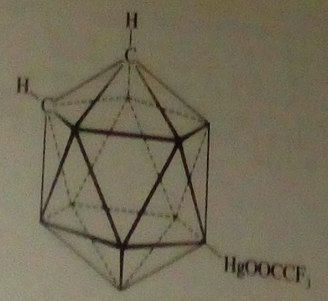
Hollander, O. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 604 (*synth, nmr, ms*)

$C_4H_{11}B_{10}F_3HgO_2$ IC-004181

1,2-Dicarbadodecaboran(12)-9-yl(trifluoroacetato-*O*) mercury, 9Cl

o-Carboran-9-ylmercury trifluoroacetate

[59993-34-9]



M 456.8

Cryst. (C_6H_6/hexane). Mp 160-162°.

Bregadze, V.I. *et al, J. Organomet. Chem.*, 1976, **112**, 249; 1977, **136**, 281 (*synth*)

$C_4H_{11}B_{10}F_3HgO_2$ IC-004182

1,7-Dicarbadodecaboran(12)-9-yl(trifluoroacetato-*O*) mercury, 9Cl

m-Carboran-9-ylmercury trifluoroacetate

[59993-35-0]

As Chloro-1,7-dicarbadodecaboran(12)-9-ylmercury, IC-003342 with

$R = -HgOOCCF_3$

M 456.8

Cryst. (C_6H_6/hexane). Mp 117-118°.

Bregadze, V.I. *et al, J. Organomet. Chem.*, 1976, **112**, 249; 1977, **136**, 281 (*synth*)

$C_4H_{11}B_{10}F_3HgO_2$ IC-004183

(1,12-Dicarbadodecaboran(12)-2-yl)(trifluoroacetato-*O*) mercury, 10Cl

p-Carboran-2-ylmercury trifluoroacetate

[64616-58-6]

As Chloro-1,12-dicarbadodecaboran(12)-2-ylmercury, IC-003343 with

$R^1 = H, R^2 = -HgOOCCF_3$

M 456.8

Cryst. (C_6H_6/hexane). Mp 226-228°.

Bregadze, V.I. *et al, J. Organomet. Chem.*, 1977, **136**, 281 (*synth*)

$C_4H_{11}FNO_2P$ IC-004184

Ethyl dimethylphosphoramidofluoridate, 9CI, 8CI

(Dimethylamido)ethoxyfluorooxophosphorus(V)

[358-29-2]

$Me_2NPF(O)OEt$

M 155.1

▷ TB4710000.

(±)-form

Liq. Bp_{18} 76-78°.

▷ V. toxic. Miotic.

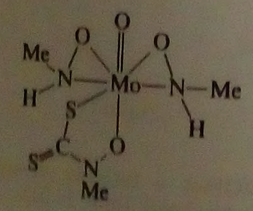
Cook, H.G. *et al, J. Chem. Soc.*, 1949, 2921 (*synth, tox*)
Mager, P.P., *Toxicol. Lett.*, 1982, **11**, 67 (*tox*)

$C_4H_{11}MoN_3O_4S_2$ IC-004185

Bis(*N*-methylhydroxylamido-*O*,*N*)*N*-methyl-*N*-oxodithiocarbamato-*O*,*S*-oxomolybdenum(*VI*)

Bis(N-*hydroxymethanaminato*-N,O)[*hydroxymethylcarbamodithioato*(2−)-O,S] *oxomolybdenum*(VI), *10Cl*

[77593-48-7]



M 325.2

Approx. pentagonal bipyramidal. Red cryst. Sol. MeOH, EtOH, MeCN, Me_2CO; insol. H_2O.

Holzbach, W. *et al, Z. Naturforsch., B*, 1981, **36**, 289 (*synth, cryst struct, ir*)

$C_4H_{11}O_2P$ IC-004186

Diethyl phosphonite, 9CI

Diethoxophosphane. Diethoxohydridophosphorus(III)

[20502-85-6]

$(EtO)_2PH$

M 122.1

Stable in Et_2O at −20°. Cannot be isol. pure.

Nifant'ev, E.E. *et al, Zh. Obshch. Khim.*, 1976, **46**, 1184; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1976, **46**, 1167 (*P-31 nmr*)
Gallagher, M.J. *et al, Aust. J. Chem.*, 1980, **33**, 287.
Nifant'ev, E.E. *et al, Tetrahedron*, 1981, **37**, 3183 (*cmr*)

$C_4H_{11}O_2PS$ IC-004187

***O,O*-Diethyl phosphonothioate, 9CI**

O,O-Diethyl thiophosphite.
Diethoxohydridothiophosphorus(V).
Diethoxo(hydrogensulfido)phosphorus(III)

[999-01-9]

$(EtO)_2P(S)H \rightleftharpoons (EtO)_2PSH$

M 154.1

Tautomeric but exists almost completely in thiophosphoryl form. Liq. with strong, sickly odour. d_4^{20} 1.07. Bp_{20} 83-84°. pK_a 8.65 (50% EtOH aq., 25°). n_D^{20} 1.4594.

Murav'ev, I.V. *et al, Zh. Obshch. Khim.*, 1968, **38**, 133; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1968, **38**, 133 (*synth*)
Nifant'ev, E.E. *et al, Zh. Obshch. Khim.*, 1983, **53**, 2695; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1983, **53**, 2429 (*synth, P-31 nmr*)

$C_4H_{11}O_2PSSe$ IC-004188

***O,O*-Diethyl phosphoroselenothioate, 9CI, 8CI**

O,O-*Diethyl phosphoroselenothioic acid.* O,O-*Diethyl hydrogen phosphoroselenothioate.* O,O-*Diethyl selenothiophosphate. Diethoxo(hydrogensulfido) selenophosphorus*(V). *Diethoxo(hydrogenselenido) thiophosphorus*(V)

[10565-43-2]

$(EtO)_2P(Se)SH \rightleftharpoons (EtO)_2P(S)SeH$

M 233.1

Exists preferentially in the thiol form. Unstable acid, isol. as K salt.

K salt: [15887-56-6].
Hygroscopic needles (Me_2CO/C_6H_6/pet. ether). Mp 169° (156° dec.). Slowly liberates Se.
Cyclohexylammonium salt: [13106-27-9].
Needles (C_6H_6/pet. ether). Mp 98-99°.

Zemlyanskii, N.I. *et al, Zh. Obshch. Khim.*, 1966, **36**, 1240; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1966, **36**, 1255 (*synth*)
Krawiecki, C. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1969, **43**, 869 (*synth*)
Stec, W.J. *et al, Phosphorus*, 1972, **2**, 97 (*P-31 nmr*)
Markowska, A. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1973, **21**, 537 (*synth*)
Bruzik, K. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1980, **54**, 141 (*synth, P-31 nmr*)
Mel'nik, Ya.I. *et al, Zh. Obshch. Khim.*, 1986, **56**, 1059; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1986, **56**, 930 (*synth*)

$C_4H_{11}O_2PS_2$ IC-004189

***O,O*-Diethyl phosphorodithioate, 9CI, 8CI**

O,O-*Diethyl dithiophosphate.* O,O-*Diethyl dithiophosphoric acid. Diethoxo(hydrogensulfido)thiophosphorus*(V)

[298-06-6]

$(EtO)_2P(S)SH$

M 186.2

Extractant for As(*III*) or Sb(*III*) in hexane from acid soln.; and also Bi(*III*) and Sb(*III*) in EtOAc/1*M* $HClO_4$ in the presence of Sn(*II*), Cu(*II*), Pb(*II*), Cd(*II*), Zn(*II*) and Tl(*I*). Liq. d_4^{20} 1.17. Bp_9 92-94°, Bp_1 60°. pK_{a1} 2.84 (EtOH), pK_{a1} 1.62 (7% EtOH aq., 20°). n_D^{20} 1.5120, 1.5070.

▷ TD7350000.

Na salt: [3338-24-7]. *Hostaflot*
Used in flotation of U and Cd ores.
▷ TD8550000.

K salt: [3454-66-8].
Cryst. (EtOH/Et_2O). Mp 152-153°, Mp 195°.
NH_4 salt: [1068-22-0].
Employed for detn. of Ni in presence of other metals.
Cryst. Mp 164-166°.
▷ BP8145000.
Et_2NH_2 salt: [39857-88-0].
Cryst. (C_6H_6/pet. ether). Mp 83-85°.
Morpholinium salt: Solid. Mp 79-81°.

Kabachnik, M.I. *et al, Tetrahedron*, 1960, **9**, 10 (*synth*)
Zemlyanskii, N.I. *et al, Zh. Obshch. Khim.*, 1960, **30**, 4056; 1972, **42**, 54; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1960, **30**, 4018; 1972, **42**, 50 (*raman, synth*)
Nyquist, R.A., *Spectrochim. Acta, Part A*, 1969, **25**, 47 (*ir*)
Jowitt, R.N. *et al, J. Chem. Soc. A*, 1970, 1702 (*ir, pmr, complexes*)
Khaskin, B.A. *et al, Zh. Obshch. Khim.*, 1973, **43**, 1916; 1974, **44**, 95; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1973, **43**, 1901; 1974, **44**, 93 (*salts*)
Olah, G.A. *et al, J. Org. Chem.*, 1975, **40**, 2582 (*props, P-31 nmr*)
Lefferts, J.L. *et al, Inorg. Chem.*, 1980, **19**, 1662 (*synth, complexes*)
Chattopadhyay, S. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1981, **24**, 27 (*pe*)
Toropova, V.F. *et al, Zh. Anal. Khim.*, 1984, **39**, 1238; *J. Anal. Chem. USSR* (*Engl. Transl.*), 1984, **39**, 988 (*props, use*)
Hayashi, K. *et al, Anal. Sci.*, 1986, **2**, 347 (*props, use*)
Fillippova, E.A. *et al, Zh. Prikl. Spektrosk.*, 1988, **49**, 454; *J. Appl. Spectrosc. USSR* (*Engl. Transl.*), 1988, **49**, 952 (*ir, raman*)

$C_4H_{11}O_2PSe$ IC-004190

***O,O*-Diethyl phosphonoselenoate, 9CI**

O,O-*Diethyl phosphoroselenoite.*
Diethoxohydridoselenophosphorus(V).
Diethoxo(hydrogenselenido)phosphorus(III)

[23416-28-6]

$(EtO)_2P(Se)H \rightleftharpoons (EtO)_2PSeH$

M 201.0

Tautomeric. Liq. d_4^{25} 1.37. $Bp_{1.2}$ 46-47°. n_D^{25} 1.4965.

Kuznetsov, E.V. *et al, CA*, 1958, **52**, 8938.
McFarlane, W. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2162 (*pmr, P-31, Se-77 nmr*)

$C_4H_{11}O_3P$ IC-004191

Diethyl phosphonate, 9CI

Diethyl phosphite. Diethoxo(hydrido)oxophosphorus(V). *Diethoxo(hydroxo)phosphorus*(III)

[762-04-9]

$(EtO)_2P(O)H \rightleftharpoons (EtO)_2POH$

M 138.1
Tautomeric. Ethylating agent for *N*-heterocyclic compds. *S*-ethylates thioamides. Hydrophosphorylating agent for alkenes and alkynes. Colourless liq. d_0^{20} 1.074. Bp 187-188°, Bp_7 50-51°. n_D^{20} 1.4076.

▷ TG7875000.

McCombie, H. *et al*, *J. Chem. Soc.*, 1945, 380 (*synth*)
Meyrick, C.I. *et al*, *J. Chem. Soc.*, 1950, 225 (*ir, raman*)
Fox, R.B. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 3967 (*deriv*)
Harless, H.R., *Anal. Chem.*, 1961, **33**, 1387 (*ms*)
Luz, Z. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 4513 (*pmr*)
Moedritzer, K., *J. Inorg. Nucl. Chem.*, 1962, **22**, 19 (*P-31 nmr*)
Hayashi, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 1510 (*props, use*)
Ovchinnikov, V.V. *et al*, *Zh. Obshch. Khim.*, 1978, **48**, 2424; *J. Gen. Chem. USSR (Engl. Transl.)*, 1978, **48**, 2199 (*P-31 nmr, tautom*)
Guthrie, P.J. *et al*, *Can. J. Chem.*, 1979, **57**, 236 (*tautom*)
Zverev, V.V. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1979, 84; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1979, 74 (*pr*)
Sidky, M.M. *et al*, *Org. Prep. Proced. Int.*, 1982, **14**, 225 (*use*)
Shagidullin, R.R. *et al*, *Dokl. Akad. Nauk SSSR*, 1987, **296**, 669; *Dokl. Phys. Chem. (Engl. Transl.)*, 1987, **296**, 939 (*ir*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1244

$C_4H_{12}AlO^{\ominus}$ IC-004192

Trihydro-*tert*-butoxyaluminate(1 –)
Trihydro(2-methyl-2-propanolato)aluminate(1 –)

$[Al[OC(CH_3)_3]H_3]^{\ominus}$

M 103.1 (ion)
From $LiAlH_4$ and $(H_3C)_3COH$ in Et_2O. Widely used stereoselective reducing agent in org. chem.
Li salt: [24507-64-0].
$C_4H_{11}AlLiO$ M 110.0
From $LiAlH_4$ and $(H_3C)_3COH$ in Et_2O. Widely used stereoselective reducing agent in org. chem. Used *in situ*. Related species $[AlH(O^tBu)_3]^{\ominus}$ and $[AlH(OMe)_3]^{\ominus}$ also descr.

Abdul Kader, M.H., *Chem. Ber.*, 1970, **103**, 1225 (*synth, ir*)
Ashby, E.C. *et al*, *J. Org. Chem.*, 1971, **36**, 197 (*use*)
Malek, J. *et al*, *Synthesis*, 1972, 217 (*rev*)
Ashby, E.C. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 3158 (*synth, props, ir*)
Horne, D.A., *J. Am. Chem. Soc.*, 1980, **102**, 6011 (*synth, pmr, cmr, Li-7 and Al-27 nmr*)
McMahon, R.J. *et al*, *J. Org. Chem.*, 1981, **46**, 99 (*use*)
Hermánek, S. *et al*, *Z. Naturforsch., B*, 1987, **42**, 539 (*ir*)

$C_4H_{12}AlO_2^{\ominus}$ IC-004193

Diethoxydihydroaluminate(1 –)

$[AlH_2(OEt)_2]^{\ominus}$

M 119.1 (ion)
Many similar species descr. It is not clear whether these are pure compds.
Li salt: [19582-13-9].
Synth. from $LiAlH_4$ + EtOH in Et_2O. White moisture-sensitive solid (Et_2O). May be a mixt. of $LiAlH_4$ and $LiAl(OEt)_4$.
Na salt: [29249-29-4].
Synth. from $NaAlH_4$ and EtOH in THF. White moisture-sensitive solid (THF). May be a mixt. of $NaAlH_4$ and $NaAl(OEt)_4$.

Abdel Kader, M.H., *Chem. Ber.*, 1970, **103**, 1225 (*ir*)
Fusek, J. *et al*, *Collect. Czech. Chem. Commun.*, 1976, **41**, 187 (*ir*)
Štrouf, O. *et al*, *Acta Chem. Scand., Ser. A*, 1977, **31**, 391 (*similar compds*)
Turova, N.Ya. *et al*, *Inorg. Chim. Acta*, 1977, **21**, 157.
Turova, N.Ya. *et al*, *Zh. Obshch. Khim.*, 1977, **47**, 1338.
Brown, H.C. *et al*, *J. Org. Chem.*, 1987, **52**, 5406 (*use*)
Hermanek, S. *et al*, *Z. Naturforsch., B*, 1987, **42**, 539 (*ir*)

$C_4H_{12}AlO_4^{\ominus}$ IC-004194

Tetramethoxyaluminate(1 –)

$[Al(OMe)_4]^{\ominus}$

M 151.1 (ion)
Homologous spp. also known.
Li salt: [28237-83-4].
Synth. from $LiAlH_4$ and MeOH in Et_2O. White moisture sensitive solid. Insol. Et_2O, THF.
Na salt: [14640-16-5].
Synth. from $NaAlH_4$ and MeOH in THF. White moisture sensitive solid. Insol. Et_2O, THF.
Cs salt: [62559-99-3].
Synth. from $CsAlH_4$ and MeOH in diglyme. White solid. Insol. Et_2O, THF.

Turova, N.Ya. *et al*, *Inorg. Chim. Acta*, 1977, **21**, 157.
Turova, N.Ya. *et al*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1977, **47**, 1231 (*synth, props, ir, powder struct*)
Turova, N.Ya. *et al*, *Koord. Khim.*, 1977, **3**, 1296 (*reactions*)
Karpovskaya, M.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 766 (*phase diagram, soly, related compds*)

$C_4H_{12}Al_8NNa_7O_{72}Si_{28}$ IC-004195

Zeolite omega
Zeolite Ω. Mazzite

$(Me_4N)Na_7[Al_8Si_{28}O_{72}]$

M 2389.2
First example of a synthetically produced zeolite subsequently found in nature. Zeolite struct. MAZ. Struct. consists of two sets of perpendicular 1-D channels (740 and 340 × 560 pm across). Synth. from Na_2O—Al_2O_3—SiO_2—H_2O—Me_4NBr gels. Occurs as rare mineral in France. Use for adsorption of small molecules. White fibres or spherulites. Dihydrated form stable at 750°. Na often replaced by K. Void vol. 0.38 $cm^3\ cm^{-3}$.

Aiello, R. *et al*, *J. Chem. Soc. A*, 1970, 1470 (*synth, powder struct*)
Breck, D.W., *Zeolite Molecular Sieves*, Wiley, 1974, 60, 167.
Rinaldi, R. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1603.
Araya, A. *et al*, *Zeolites*, 1984, **4**, 263 (*synth*)
Jones, N. *et al*, *J. Am. Chem. Soc.*, 1985, 6767 (*Si-29 nmr*)
Newsam, J.M. *et al*, *Mater. Res. Bull.*, 1985, **20**, 125.
Fyfe, C.A. *et al*, *Zeolites*, 1985, **5**, 179 (*Si-29, Al-27 nmr*)
Meier, W.M. *et al*, *Atlas of Zeolite Structure Types*, 2nd Ed., Butterworth, London, 1987, 92.
Fajula, F. *et al*, *Zeolites*, 1987, **7**, 203 (*synth*)
Massiani, P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 814 (*Al-27 nmr*)

$C_4H_{12}AsClN_2$ IC-004196

Chlorobis(dimethylamino)arsine
Tetramethylarsenodiamidous chloride, 11Cl.
Chlorobis(dimethylamido)arsenic
[80489-42-5]

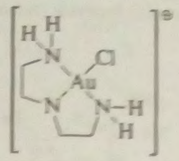
$(Me_2N)_2AsCl$

M 198.5
Liq. d_4^{20} 1.35. Bp_{10} 69-70°. n_D^{20} 1.5247.

Kamai, G. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1955, **105**, 489 (*synth*)
Vetter, H.-J., *Naturwissenschaften*, 1964, **51**, 240 (*pmr*)
Vetter, H.-J. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **330**, 233 (*synth*)

$C_4H_{12}AuClN_3^{\ominus}$ IC-004197

[Bis(2-aminoethyl)amido]chlorogold(*III*)(1 +)
[N-(2-Aminoethyl)-1,2-ethanediaminato-N,N',N'']chlorogold(III)(1 +), 10Cl



M 334.5 (ion)
Perchlorate: [73440-05-8].
Light yellow cryst. (H_2O).
▷ Potentially explosive.

Nardin, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 220 (*synth, cryst struct*)

$C_4H_{12}B^{\ominus}$ IC-004198

***tert*-Butyltrihydroborate**
(1,1-Dimethylethyl)trihydroborate(1 –), 10Cl. tert-Butylborohydride

$[(H_3C)_3CBH_3]^{\ominus}$

M 70.9 (ion)
Li salt: [76826-51-2].
$C_4H_{12}BLi$ M 77.8
Air- and moisture-sensitive.

Biffar, W. *et al*, *Chem. Ber.*, 1981, **114**, 49 (*pmr, nmr*)

$C_4H_{12}BBr_2P$ IC-004199

Dibromomethyl(trimethylphosphine)boron, 10Cl
Dibromomethylborane trimethylphosphine.
Methyldibromoborane trimethylphosphine
[69513-15-1]

$Me_3P{-}BBr_2Me$

M 261.7
Solid. Mp 236-237°.

Martin, D.R. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1289 (*synth, pmr*)

$C_4H_{12}BNO$ IC-004200

Trihydro(morpholine-N^4)boron, 10Cl
Borane morpholine. Morpholine compd. with borane(1:1), 9Cl, 8Cl. Morpholine borane
[4856-95-5]

As Trifluoro(morpholine-N^4)boron, IC-004108 with

X = H

M 100.9
Used in photographic colour processing. Preservative for metal-working fluid. Shows anticholesteremic, hypolipidemic and antiflammatory activity. Commercially available. Cryst. (H_2O). Mp 82-85°, Mp 97-99°.

▷ Toxic. QD8530000.

U.S. Pat., 2 927 133, (1960); *CA*, **55**, 3433i.
Hill, E.A. *et al*, *Tetrahedron Lett.*, 1976, 3013.
Bennett, E.O. *et al*, *Mater. Perform.*, 1979, **18**, 40 (*use*)
Hall, I.H. *et al*, *J. Pharm. Sci.*, 1981, **70**, 339 (*use*)
Wilson, I. *et al*, *Inorg. Chem.*, 1982, **21**, 1622.
U.S. Pat., 4 312 989, (1982); *CA*, **97**, 85322g.

$C_4H_{12}B_2Cl_2N_2$ IC-004201

1,2-Dichloro-1,2-bis(dimethylamino)diborane(4)
1,2-Dichloro-N,N,N',N'-tetramethyl-1,2-diborane(4)-diamine, 10Cl
[64541-76-0]

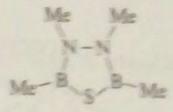
$Me_2NBCl{-}BClNMe_2$

M 180.6
Thermally stable oil, can be kept at 20° for several weeks in inert atm., moisture-sensitive. d_{22} 1.079. Bp_1 57-60°, $Bp_{0.1}$ 34-35°. n_D^{20} 1.4728.

Nöth, H. *et al*, *Z. Naturforsch., B*, 1962, **17**, 714 (*synth, props*)
Brown, M.P. *et al*, *Chem. Ind. (London)*, 1963, 85.
Nöth, H. *et al*, *J. Organomet. Chem.*, 1964, **1**, 401 (*synth*)
Kiesmeier, B. *et al*, *Chem. Ber.*, 1977, **110**, 2774 (*nmr*)
Gundersen, G., *CA*, 1978, **89**, 93257a (*struct*)
Biffar, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1980, **19**, 56 (*props*)

$C_4H_{12}B_2N_2S$ IC-004202

2,3,4,5-Tetramethyl-1,3,4,2,5-thiadiazadiborolidine, 10Cl
2,3,4,5-Tetramethyl-1,3,4,2,5-thiadiazaborolane
[40392-37-8]



M 141.8
Low melting cryst., sensitive to air and moisture. Sol. non-hydroxylic solvs. Mp 13°.

Nölle, D. *et al*, *Z. Naturforsch., B*, 1972, **27**, 1425 (*synth*)
Kroner, J. *et al*, *Chem. Ber.*, 1975, **108**, 3807 (*pe*)
Fünstetter, H. *et al*, *Chem. Ber.*, 1980, **113**, 3881 (*struct, props*)
Barlos, K. *et al*, *Z. Naturforsch., B*, 1980, **35**, 125 (*props*)

$C_4H_{12}B_2O_4$ IC-004203

Tetramethoxydiborane(4), 10Cl, 9Cl, 8Cl
[7318-94-7]

$(MeO)_2B{-}B(OMe)_2$

M 145.7
Liq., v. sensitive to moist air; thermally stable to ca. 110° *in vacuo*. Mp −26°. Bp_{25} 46-47°. n_D^{20} 1.4075.

Brotherton, R.J. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 6245 (*synth, props*)
Nöth, H. *et al*, *Chem. Ber.*, 1961, **94**, 509; 1966, **99**, 1049; 1981, **114**, 3044 (*synth, nmr, props*)
Becher, H.J. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **314**, 226 (*ir, raman, struct*)
Brubaker, G.L. *et al*, *Inorg. Chem.*, 1969, **8**, 2804 (*ms*)

$C_4H_{12}B_4$ IC-004204

2,3-Dimethyl-2,3-dicarbahexaborane(8), 10Cl
[20741-68-8]

As 2,3-Dicarbahexaborane(8), IC-003255 with

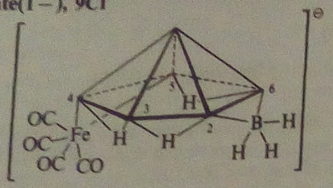
$R^1 = R^2 = CH_3$

M 103.3
Colourless liq. by vacuum fractionation. Mp −64°.

Onak, T. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 3378 (*synth, nmr*)
Boer, F. *et al*, *Inorg. Chem.*, 1964, **3**, 1666 (*struct*)
Jotham, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 473 (*ir, raman*)
Grimes, R. *et al*, *Inorg. Chem.*, 1979, **18**, 3294 (*synth*)

$C_4H_{12}B_7FeO_4^{\ominus}$ IC-004205

Tetracarbonyl[η^2-dodecahydroheptaborato(1−)]ferrate(1−), 9CI



M 255.6 (ion)

Tetrabutylammonium salt: [54083-17-9].
Deep-amber cryst. (CH_2Cl_2/pentane).

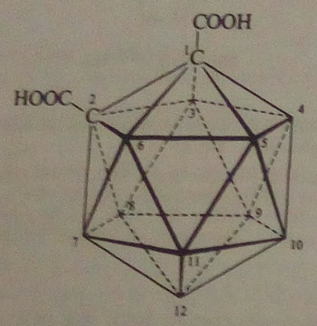
Hollander, O. *et al*, *J. Chem. Soc., Chem. Commun.*, 1974, 604 (*synth, struct*)
Mangion, M. *et al*, *Inorg. Chem.*, 1977, **16**, 2110 (*struct*)

$C_4H_{12}B_{10}O_4$ IC-004206

1,2-Dicarbadodecaborane(12)-1,2-dicarboxylic acid

1,2-Dicarboxy-1,2-dicarbadodecaborane(12). o-*Carboranedicarboxylic acid*

[23835-80-5]



M 232.2

closo-. Precursor to carborane polymers. White solid (toluene). Mp 232° (223-225°).

Heying, T.L. *et al*, *Inorg. Chem.*, 1963, **2**, 1097 (*synth*)
Grafstein, D. *et al*, *Inorg. Chem.*, 1963, **2**, 1120 (*synth*)

$C_4H_{12}B_{10}O_4$ IC-004207

1,7-Dicarbadodecaborane(12)-1,7-dicarboxylic acid, 10CI

1,7-Dicarboxy-1,7-dicarbadodecaborane(12). m-*Carboranedicarboxylic acid*

[50571-15-8]

M 232.2

closo-. Precursor to carborane polymers. White solid (CH_2Cl_2). Mp 207°. pK_a 6.8.

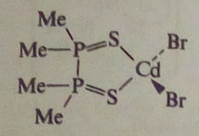
Grafstein, D. *et al*, *Inorg. Chem.*, 1963, **2**, 1129 (*synth*)
Rabilloud, G. *et al*, *J. Organomet. Chem.*, 1979, **182**, 275 (*synth, ir, ms*)

$C_4H_{12}Br_2CdP_2S_2$ IC-004208

Dibromo(tetramethyldiphosphine-1,2-disulfide-*S,S'*)cadmium, 10CI

(*Tetramethyldiphosphine-1,2-disulfide*-S,S')*cadmium dibromide. Cadmium*(II) *bromide* (*tetramethyldiphosphine-1,2-disulfide*)

[71231-55-5]



M 458.4
Symmetry: C_{2v}. Unstable solid.

McQuillan, G.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 895 (*synth, ir, raman*)

$C_4H_{12}Br_2CuO_2S_2$ IC-004209

Dibromobis(dimethyl sulfoxide)copper(*II*)

Dibromo(*methyl sulfoxide*)*copper, 8CI. Dibromo*[*sulfinylbis*[*methane*]-O]*copper, 9CI. Copper*(II) *bromide bis*(*dimethyl sulfoxide*)

[59448-49-6]

$CuBr_2(O{=}SMe_2)_2$

M 379.6
Square pyramidal geometry around Cu with 2 short Cu—Br contacts (243, 245 pm) and a further Cu—Br contact between formula units (278 pm) at the axial position giving a homopolymer. Synth. by addition of DMSO to anhydrous $CuBr_2$ in EtOH. Orange cryst. or dark brown platelets (DMSO). Insol. EtOH. Mp 115° dec.

[65914-13-8, 65914-14-9]

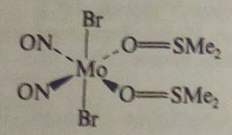
Selbin, J. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **16**, 219 (*synth*)
Holah, D.K. *et al*, *Inorg. Chem.*, 1965, **4**, 1721 (*magnetism*)
Willett, R.D. *et al*, *Inorg. Chim. Acta*, 1977, **25**, 97 (*cryst struct*)

$C_4H_{12}Br_2MoN_2O_4S_2$ IC-004210

Dibromobis(dimethyl sulfoxide)dinitrosylmolybdenum

Dibromodinitrosylbis[*sulfinylbis*[*methane*]-O]*molybdenum, 11CI*

[89247-92-7]



M 472.0
Distorted octahedral. Synth. from $MoBr_2(NO)_2$ and DMSO in CH_2Br_2. Green cryst.

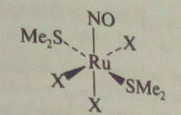
Schumacher, C. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **508**, 79 (*cryst struct, synth, ir*)

$C_4H_{12}Br_3NORuS_2$ IC-004211

Tribromobis(dimethyl sulfide)(nitrosyl)ruthenium

Tribromo(*nitrosyl*)*bis*[*thiobis*[*methane*]]*ruthenium, 9CI*

[61567-04-2]



X = Br

M 495.0
Single *mer,trans*-octahedral isomer obsd. Prepared by treating an NO-saturated EtOH soln. of $RuBr_3{\cdot}xH_2O$ with SMe_2. Red-brown solid. Ir ν_{NO} 1872; ν_{RuBr} 275, 236 cm^{-1}.

Fergusson, J.E. *et al*, *Aust. J. Chem.*, 1976, **29**, 2159 (*synth, ir, uv, pmr, cmr*)

$C_4H_{12}Br_4MoS_2^{\ominus}$ IC-004212

Tetrabromobis(dimethyl sulfide)molybdate(*III*)(1−)

Tetrabromobis[*thiobis*[*methane*]]*molybdate*(III)(*1−*), *11CI*

$[MoBr_4(SMe_2)_2]^{\ominus}$

M 539.8 (ion)
trans-Octahedral anion.

Trimethylsulfonium salt: [96342-01-7].
Synth. by reaction of $MoBr_4$ and excess Me_2S. Red cryst.

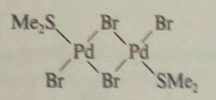
Schumacher, C. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **520**, 25 (*cryst struct, synth, ir*)

$C_4H_{12}Br_4Pd_2S_2$ IC-004213

Tetrabromobis(dimethyl sulfide)dipalladium(*II*)

Di-μ-bromodibromobis(*methyl sulfide*)*dipalladium, 8CI. Di-μ-bromodibromobis*[*thiobis*(*methane*)]*dipalladium, 9CI*

[21315-76-4]



M 656.7
Has 2 Br bridges in square planar *trans*-configuration. Contrast Pt analogue (Tetrabromobis(diethyl sulfide) diplatinum(*II*), IC-006170) which is S-bridged. More stable than Se, Te analogues. Synth. from $Pd(SMe_2)_2Br_2$ in EtOH or Tetrachloropalladate(*II*)(2−), IC-017115 + SMe_2. Monoclinic prisms. Sol. CH_2Cl_2, MeOH. Mp 169°.

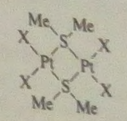
Sales, D.L. *et al*, *J. Chem. Soc. A*, 1968, 1852 (*struct*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1904 (*synth, ir, pmr*)
Lobaneva, O.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1972, **17**, 1583; 1975, **20**, 1577 (*ir*)

$C_4H_{12}Br_4Pt_2S_2$ IC-004214

Tetrabromobis(μ-dimethyl sulfide)diplatinum(*II*), 8CI

Tetrabromobis[*μ-thiobis*[*methane*]]*diplatinum*(II), *9CI*

[20004-38-0]



X = Br

M 834.0
Structure with bridging sulfides deduced from ir and raman spectra. Synth. from Tetrabromoplatinate(*II*)(2−), IC-002066 + $[PtBr_2(SMe_2)_2]$. Yellow solid. Sol. CH_2Cl_2. Mp 190-195° dec. Similar compds. known for Cl, other SR_2.

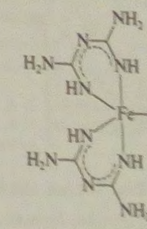
Monomer: Dibromo(*dimethyl sulfide*)*platinum*(II)
$C_2H_6Br_2PtS$ M 417.0
Has no separate existance.

Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 576 (*synth*)

$C_4H_{12}ClFeN_{10}^{\ominus}$ IC-004215

Chlorobis(imidodicarbonimidic diamidato-*N'',N'''*)iron

Bis(*biguanidinato*)*chloroiron*



M 291.5 (ion)
Spin quartet ground state of Fe(*III*).

Monohydrochloride: [77648-28-3].
$C_4H_{12}Cl_2FeN_{10}$ M 326.9
Synth. from anhyd. $FeCl_3$ + ligand in Me_2CO. Pale brown solid; air-stable. Insol. most org. solvs.

Lahiry, S. *et al*, *Inorg. Chem.*, 1981, **20**, 2789 (*synth, mössbauer, magnetism*)

$C_4H_{12}ClGaN_2$ IC-004216

Chlorobis(dimethylamido)gallium(*III*)

$[GaCl(NMe_2)_2]_2$

M 193.3
Dimeric.

Dimer: [57776-77-9]. *Dichlorotetrakis*(*dimethylamido*)*digallium*(III). *Dichlorotetrakis*(*N-methylmethanaminato*)*digallium, 9CI*
$C_8H_{24}Cl_2Ga_2N_4$ M 386.6
Synth. from $GaCl_3$ and $LiNMe_2$. V. air- and moisture-sensitive colourless cryst. (pentane). Sol. hexane, C_6H_6, Et_2O. Mp 60-61°. Isomers in soln. detected by nmr.

Nöth, H. *et al*, *Z. Naturforsch., B*, 1975, **30**, 681 (*synth, pmr, ir*)

$C_4H_{12}ClN_2OP$ IC-004217

Tetramethylphosphorodiamidic chloride, 9CI

Bis(dimethylamino) phosphoryl chloride. Bis(dimethylamino) phosphinic chloride. Chlorobis(dimethylamido) oxophosphorus(V)

[1605-65-8]

$(Me_2N)_2P(O)Cl$

M 170.5

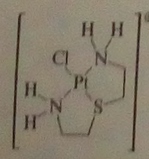
Liq. d_4^{20} 1.823. Bp_{30} 133-134°, Bp_{10} 110°, $Bp_{0.6}$ 79-82°. n_D^{25} 1.4661.

Nielsen, M.L. *et al, J. Phys. Chem.*, 1964, **68**, 152 (*P-31 nmr*)
Cowley, A.H. *et al, J. Am. Chem. Soc.*, 1965, **87**, 4451 (*pmr*)
Traylor, P.S. *et al, J. Am. Chem. Soc.*, 1965, **87**, 553 (*props*)
Keat, R. *et al, J. Chem. Soc. A*, 1968, 703 (*pmr*)
Köttgen, D. *et al, Z. Anorg. Allg. Chem.*, 1971, **385**, 56 (*ir, raman*)
Osokin, D.Ya. *et al, Org. Magn. Reson.*, 1972, **4**, 831 (*nqr*)
Laskorin, B.N. *et al, Dokl. Akad. Nauk SSSR*, 1974, **215**, 595; *Dokl. Phys. Chem. (Engl. Transl.)*, 1974, **215**, 174 (*ir, P-31 nmr, pmr*)
Zverev, V.V. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1975, 1051; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1975, 961 (*pe*)
Poignant, S. *et al, Can. J. Chem.*, 1980, **58**, 946 (*pmr, P-31 nmr*)

$C_4H_{12}ClN_2PtS^{\oplus}$ IC-004218

Chloro[bis(2-aminoethyl) sulfide]platinum(*II*)

Chloro[2,2'-thiobis(ethanamine)]platinum(1+), *10CI*



M 350.7 (ion)

Ring system strained. Relat. compds. also known.

Chloride. [71853-03-7]

$C_4H_{12}Cl_2N_2PtS$ M 386.2

Yellow-white solid.

Albertin, G. *et al, Inorg. Chem.*, 1979, **18**, 1451.

$C_4H_{12}ClN_2Sb$ IC-004219

Chlorobis(dimethylamino)stibine

1-Chloro-N,N,N',N'-tetramethylstibinediamine, 11CI. Chlorobis(dimethylamido)antimony

[95688-59-8]

$(Me_2N)_2SbCl$

M 245.3

Yellow cryst. Mp *ca.* 140° dec.

Ensinger, U. *et al, Z. Anorg. Allg. Chem.*, 1984, **514**, 137; 1985, **520**, 160 (*synth, ir, pmr, ms*)

$C_4H_{12}Cl_3CrN_2$ IC-004220

Dichloro(2-methyl-1,2-propanediamine)chromium(*II*), 8CI

Dichloro(1,2-diamino-2-methylpropane)chromium(II)

[33826-34-5]

$CrCl_2[H_2NC(CH_3)_2CH_2NH_2]$

M 211.0

6-Coordinate, chloride bridged polymer. Light blue, air-sensitive solid. μ_{eff} = 4.02μ_B (300K); 2.67μ_B (90K).

Larkworthy, L.F. *et al, J. Chem. Soc. A*, 1971, 2766 (*synth, props*)

$C_4H_{12}Cl_2CrO_2S_2$ IC-004221

Dichlorobis(dimethyl sulfoxide)chromium(*II*)

Dichlorobis(methyl sulfoxide)chromium. Chromium(II) *chloride bis(dimethyl sulfoxide)*

$[CrCl_2(O{=}SMe_2)_2]_n$

M 279.1

Chloride-bridged polymer with distorted octahedral Cr(*II*). Pale blue cryst. (EtOH). μ_{eff} = 4.91μ_B (293K).

Holah, D.G. *et al, Inorg. Chem.*, 1965, **4**, 1721 (*synth, uv, ir*)

$C_4H_{12}Cl_2CuO_2S_2$ IC-004222

Dichlorobis(dimethyl sulfoxide)copper(*II*)

Dichlorobis(methyl sulfoxide)copper, 8CI. Dichlorobis[sulfinylbis[methane]-O]copper, 9CI. Copper(II) *chloride bis(dimethyl sulfoxide)*

[14215-41-9]

$CuCl_2(O{=}SMe_2)_2$

M 290.7

Square pyramidal geometry around Cu with 2 short *trans* Cu—Cl contacts (229, 228 pm) and a longer Cu—Cl contact between formula units (270 pm) at the axial position giving a homopolymer. Synth. by addition of DMSO to $CuCl_2$ (anhydrous) in EtOH. Green cryst. Sol. DMSO; insol. Et_2O. Mp 125° dec.

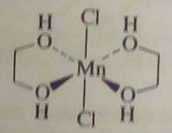
[60686-96-6]

Selbin, J. *et al, J. Inorg. Nucl. Chem.*, 1961, **16**, 219 (*synth, ir*)
Haberditzl, W. *et al, Z. Phys. A:*, 1965, **228**, 73 (*magnetism*)
Ramasubba Reddy, T. *et al, J. Chem. Phys.*, 1966, **45**, 2714 (*esr*)
Willett, R.D. *et al, Inorg. Chim. Acta*, 1970, **4**, 447 (*cryst struct*)
Su, C.-C. *et al, Inorg. Chem.*, 1974, **13**, 1734 (*esr*)
Adams, D.M. *et al, Inorg. Chem.*, 1976, **15**, 1968 (*ir*)
Estes, W.E. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 2121 (*magnetism*)

$C_4H_{12}Cl_2MnO_4$ IC-004223

Dichlorobis(ethane-1,2-diol)manganese(*II*), 9CI

[42131-18-0]



M 249.9

trans-Octahedral. Prepd. by dissolving $MnCl_2.4H_2O$ in 1,2-ethanediol. Pink hygroscopic cryst. Mp 122-123°. Forms a monohydrate.

[52079-44-4]

Gomer, R. *et al, J. Am. Chem. Soc.*, 1944, **66**, 1331 (*hydrate*)
Antti, B.M., *Acta Chem. Scand.*, 1973, **27**, 3513 (*synth, cryst struct*)
Knetsch, D. *et al, Inorg. Chim. Acta*, 1973, **7**, 81 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **81**, 35 (*rev, bibl*)

$C_4H_{12}Cl_2N_2O_3Ru$ IC-004224

Diaquadichloro(dinitrogen)(tetrahydrofuran) ruthenium(*II*), 8CI

[18958-67-3]

$RuCl_2(OH_2)_2(THF)(N{\equiv}N)$

M 308.1

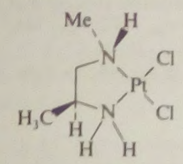
Stereochem. uncertain. Prepd. by reducing $RuCl_3.xH_2O$ in THF with Zn/Hg at −20° under N_2 (1-40 atm.). Brown solid. Dark yellow soln. in THF. Also sol. Me_2CO, EtOH, H_2O. Ir ν_{N_2} 2150 cm^{-1} (nujol); ν_{N_2} 2125 cm^{-1} (THF).

Shilov, A.E. *et al, Kinet. Katal.*, 1966, **7**, 685 (*synth*)
Borod'ko, Y.G. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1967, **176**, 927 (*synth, reactions*)
Shilova, A.K. *et al, Kinet. Katal.*, 1968, **9**, 767; 1969, **10**, 213 (*ir, N_2 exchange*)
Borod'ko, Y.G. *et al, Russ. Chem. Rev.* (*Engl. Transl.*), 1969, **38**, 355 (*rev*)
Shilov, A.E. *et al, Zh. Neorg. Khim.*, 1969, **14**, 2286 (*synth*)
Borod'ko, Y.G. *et al, Russ. J. Phys. Chem.* (*Engl. Transl.*), 1970, **44**, 349 (*synth, ir, reactions*)

$C_4H_{12}Cl_2N_2Pt$ IC-004225

Dichloro(N^1-methyl-1,2-propanediamine)platinum, 9CI

Dichloro(N-*methyl-1,2-diaminopropane*)*platinum*(II). *Dichloro*(*1-methylamino-2*(S)-*aminopropane*)*platinum*(II)



(R_N,S_C)-*form*

M 354.1

Unusual chiral square planar Pt(*II*) complex. Sl. sol. H_2O. Stereoisomers separated mechanically.

(R_N,S_C)-*form* [56258-73-2]

Yellow needles.

(S_N,S_C)-*form* [56323-56-9]

(−)-*form*

Pale yellow blocks.

Bosnich, B. *et al, Inorg. Chem.*, 1975, **14**, 2768 (*synth, uv-vis, pmr, cd*)
Ball, R.G. *et al, Inorg. Chem.*, 1976, **15**, 1704 (*cryst struct, abs config*)

$C_4H_{12}Cl_2OS_2V$ IC-004226

Dichlorobis(dimethyl sulfide)oxovanadium(*IV*)

Dichlorobis(methyl sulfide)oxovanadium(IV), *8CI*

[18661-56-8]

$VOCl_2(SMe_2)_2$

M 262.1

Prob. square pyramidal monomer: detailed geometry is not known. Synth. by reduction of $VOCl_3$ by Me_2S in *iso*-octane. Blue solid. Ir ν_{VO} 995 cm^{-1}; paramagnetic, μ_{eff} = 1.77μ_B.

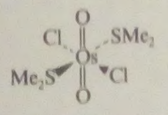
Baker, K.L. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1881 (*synth, uv-vis, ir, magnetism*)

$C_4H_{12}Cl_2O_2OsS_2$ IC-004227

Dichlorobis(dimethyl sulfide)dioxoosmium(*VI*)

Dichlorodioxobis[thiobis[methane]]osmium(VI), *11CI*

[95824-04-7]



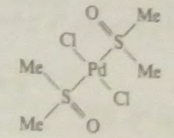
M 417.3

$C_4H_{12}Cl_2O_2PdS_2$ IC-004228

Dichlorobis(dimethyl sulfoxide)palladium(*II*)

Dichlorobis[sulfinylbis(methane)]palladium(II), *9CI. Dichlorobis(methyl sulfoxide)palladium*(II), *8CI*

[12386-08-2]



trans-S-bonded form

M 333.5

O-bonded form not positively identified, prob. non-existent. Simplest of many $PdX_2(R_2SO)_2$ complexes.

trans-O-form [14568-12-8]

trans-S-form [15274-32-5]

Orange cryst. (CH_2Cl_2/C_6H_6 or DMSO/Me_2CO). Mp 203-204°. Soln. dec. to Tetrachlorobis(dimethyl sulfoxide)dipalladium(*II*), IC-004238, but formation of *cis*-isomer claimed in MeCN.

[15280-84-9, 38929-74-7]

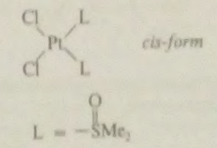
Bennett, M.J. *et al, Acta Crystallogr.*, 1967, **23**, 788 (*synth, cryst struct*)
Wayland, B.B. *et al, Inorg. Chem.*, 1969, **8**, 971 (*isomers*)
Tranquille, M. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 1305 (*synth, ir, raman*)

$C_4H_{12}Cl_2O_2PtS_2$ IC-004229

Dichlorobis(dimethyl sulfoxide)platinum(*II*)

Dichlorobis(methyl sulfoxide)platinum, 8CI. Dichlorobis[sulfinylbis(methane)-S]platinum, 9CI

[14568-13-9]



cis-form

M 422.2

cis-form [22840-91-1]

More studied than *trans* form. DMSO coordinated through S. Isom. photochemically. Yellow needles. Sol. $CHCl_3$.

trans-form [30729-25-0]

Probably coordinated by S. Prepd. from $[Pt_2Cl_4(DMSO)_2]$ + DMSO.

[15274-33-6, 25794-47-2, 39336-39-5, 75992-73-3]

Cotton, F.A. *et al, J. Phys. Chem.*, 1960, **64**, 1534 (*ir*)
Kitching, W. *et al, Inorg. Chem.*, 1970, **9**, 541 (*synth, ir, pmr*)
Melanson, R. *et al, Can. J. Chem.*, 1975, **53**, 2371 (*cryst struct*)
Price, J.H. *et al, Inorg. Chem.*, 1978, **17**, 2245 (*photochem*)
Annibale, G. *et al, Inorg. Chem.*, 1985, **24**, 797 (*trans-form*)

$C_4H_{12}Cl_2O_2V$ IC-004230

Dichlorobis(ethanol)vanadium(*II*), 11Cl

Vanadium(II) *chloride bis(ethanol)*

[86973-30-0]

$VCl_2(EtOH)_2$

M 213.9

Octahedral polymeric chain struct. Synth. from $VCl_2.2H_2O$ + equimolar EtOH/ethyl orthoformate. Pale green solid. Paramagnetic, $\mu_{eff} = 3.33\mu_B$ (295K), $2.61\mu_B$ (90K), $\theta = 113$K.

Bis-EtOH complex: see *Dichlorotetrakis(ethanol) vanadium*(II), IC-006281

Larkworthy, L.F. *et al*, *Inorg. Chim. Acta*, 1983, **71**, 81 (*synth, uv-vis, magnetism*)

$C_4H_{12}Cl_2O_4W$ IC-004231

Dichlorotetramethoxytungsten(*VI*), 9Cl

$WCl_2(OMe)_4$

M 378.8

Octahedral.

cis-form [35869-30-8]

Interatomic distances: W—O 184, W—Cl 243, 241 pm. Monomeric, *cis*-config. persists in soln. Synth. form WCl_6 + 4MeOSiMe$_3$. Pale yellow cryst. Mp 79-81°.

trans-form [35869-31-9]

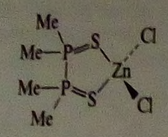
Synth. from *cis*-$W(OMe)_4F_2$ and $[(H_3C)_3C]SiCl$. Pale lemon-yellow cryst.

Handy, L.B. *et al*, *Inorg. Chem.*, 1972, **11**, 523 (*pmr, synth*)
Handy, L.B., *Acta Crystallogr., Sect. B*, 1975, **31**, 300 (*cryst struct*)

$C_4H_{12}Cl_2P_2S_2Zn$ IC-004232

Dichloro(tetramethyldiphosphine 1,2-disulfide-*S,S'*) zinc(*II*), 10Cl

[15559-88-3]



M 322.5

Air-stable cryst. Sl. sol. polar org. solvs. Dec. on heating to ZnS and diphosphine.

[71231-52-2]

Arshad, M. *et al*, *Chem. Ind. (London)*, 1964, 1181 (*synth*)
Arshad, M. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 1031 (*ir*)
McQuillan, G.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 895 (*ir, raman*)

$C_4H_{12}Cl_2PtS_2$ IC-004233

Dichlorobis(dimethyl sulfide)platinum(*II*), 8Cl

Dichlorobis[thiobis(methane)]platinum, 9Cl

As Dichlorobis(dimethyl sulfoxide)platinum(*II*), IC-004229 with

$L = SMe_2$

M 390.2

Undergoes complex equilibria in soln.

cis-form [17836-09-8]

Yellow solid. Sol. many org. solvs. Mp 159°.

trans-form [17457-51-1]

Orange solid. Sol. many org. solvs. Mp 159°.

[55449-91-7]

Cox, E.G. *et al*, *J. Chem. Soc.*, 1934, 182 (*synth, x-ray*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1904 (*synth, ir, raman*)
Roulet, R. *et al*, *Helv. Chim. Acta*, 1973, **56**, 2179 (*equilibria*)
Kennedy, J.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 874 (*nmr*)
Canovese, L. *et al*, *Inorg. Chem.*, 1981, **20**, 4166 (*synth*)
Swaddle, T.W., *Adv. Inorg. Bioinorg. Mech.*, 1983, **2**, 95.

$C_4H_{12}Cl_3NORuS_2$ IC-004234

Trichlorobis(dimethyl sulfide)(nitrosyl)ruthenium

Trichloro(nitrosyl)bis[thiobis[methane]]ruthenium, 9Cl

[61566-97-0]

As Tribromobis(dimethyl sulfide)(nitrosyl)ruthenium, IC-004211 with

$X = Cl$

M 361.7

Single *mer, trans*-octahedral isomer obsd. Prepd. by treating an NO-saturated EtOH soln. of $RuCl_3.xH_2O$ with SMe_2. Red solid. Ir ν_{NO} 1872; ν_{RuCl} 348, 332, 316 cm^{-1}.

Fergusson, J.E. *et al*, *Aust. J. Chem.*, 1976, **29**, 2159 (*synth, ir, uv, pmr, cmr*)

$C_4H_{12}Cl_4IrO_2S_2^{\ominus}$ IC-004235

Tetrachlorobis(dimethyl sulfoxide)iridate(*III*)(1−), 9Cl

Tetrachlorobis[sulfinylbis[methane]-S]iridate(1−), 9Cl

$[IrCl_4[S(O)Me_2]_2]^{\ominus}$

M 490.3 (ion)

DMSO bonds through S in both isomers.

cis-form

Isoquinolinium salt: [52645-44-0].
Tan needles. Mp 165-170°.

trans-form

H compd.: [52544-08-8].
Pink needles. Sol. DMSO. Mp 171.5-172°.

Hadelad, Y.M.Y. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1974, 592 (*synth, ir, pmr*)

$C_4H_{12}Cl_4IrS_2^{\ominus}$ IC-004236

Tetrachlorobis(dimethyl sulfide)iridate(*III*)(1−)

Tetrachlorobis[thiobis[methane]]iridate(III)(1−), *10Cl*

$[Ir(SMe_2)_2Cl_4]^{\ominus}$

M 458.3 (ion)

Octahedral geometry.

cis-form

Me_4N salt: [75674-59-8].
Purple solid. Sol. DMSO.

trans-form

Me_4N salt: [75714-86-2].
Purple solid. Sol. DMSO.

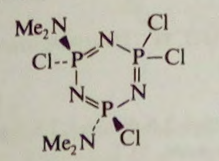
Gulliver, D.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1872 (*synth, ir, pmr*)

$C_4H_{12}Cl_4N_5P_3$ IC-004237

2,2,4,6-Tetrachloro-4,6-bis(dimethylamino)-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 9Cl

2,2,4,6-Tetrachloro-4,6-bis(dimethylamino)-2,2,4,4,6,6-hexahydrocyclotriphosphazene. 2,2,4,6-Tetrachloro-4,6-bis(dimethylamino)-2λ^5,4λ^5,6λ^5-cyclotriphosphaza-1,3,5-triene. 2,2,4,6-Tetrachloro-4,6-bis(dimethylamino)-1,3,5,2λ^5,4λ^5,6λ^5-triazatriphosphinine

[2203-74-9]



(4RS,6RS)-form

M 364.9

Cis- and *trans* forms equilibrate in soln. or in presence of $AlCl_3$.

(4RS, 6RS)-form [1081-87-4]

trans-*form*
Solid or cryst. (pet. ether). Mp 103°. Almost flat ring with sl. chair conformation.

(4RS, 6SR)-form [1018-07-1]

cis-*form*
Solid or cryst. (pet. ether). Mp 86°. Almost flat ring with sl. chair conformation.

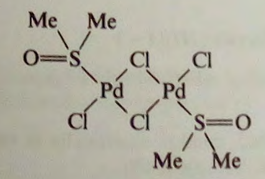
Keat, R. *et al*, *J. Chem. Soc.*, 1965, 2215 (*synth, pmr, struct*)
Strahlberg, R. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2005 (*ir, raman*)
Keat, R. *et al*, *J. Chem. Soc. A*, 1968, 703 (*pmr*)
Goldschmidt, J.M.E. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 161, 163 (*synth*)
Green, B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1042 (*pe*)
Dagleish, W.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 308 (*nqr*)
Keat, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1582 (*P-31 nmr*)
Connelly, A. *et al*, *J. Magn. Reson.*, 1978, **30**, 439 (*nqr, struct*)
Ahmed, F.R. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1456 (*cryst struct*)
Friedmann, N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 103 (*props*)
Thomas, B. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **489**, 131 (*N-14, P-31 nmr*)
Sridharan, K.R. *et al*, *Polyhedron*, 1984, **3**, 867 (*nqr*)

$C_4H_{12}Cl_4O_2Pd_2S_2$ IC-004238

Tetrachlorobis(dimethyl sulfoxide)dipalladium(*II*)

Di-μ-chlorodichlorobis(methyl sulfoxide)dipalladium, 8Cl.
Di-μ-chlorodichlorobis[sulfinylbis(methane)]dipalladium, 9Cl

[25257-82-3]



M 510.9

Probable struct. shown. Synth. from Dichlorobis(dimethyl sulfoxide)palladium(*II*), IC-004228 in $CHCl_3$ or from Bis(benzonitrile)dichloropalladium, IC-008528 + DMSO. Deep red-brown solid. Reacts with CO → $PdCl_2(CO)(DMSO)$, breaking bridged struct.

[21340-23-8]

Kitching, W. *et al*, *Inorg. Chem.*, 1970, **9**, 541 (*synth, ir*)
Andronov, E.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 1235 (*reactions*)

$C_4H_{12}Cl_4O_2RuS_2^{\ominus}$ IC-004239

Tetrachlorobis(dimethyl sulfoxide)ruthenate(*III*)(1−)

Tetrachlorobis[sulfinylbis[methane]-S]ruthenate(III)(1−), *9Cl*

[61779-26-8]

$[RuCl_4(O{=}SMe_2)_2]^{\ominus}$

M 399.1 (ion)

Both sulfoxide ligands are thought to be *S*-bonded. Prepd. by treating $[Ru(DMSO)_6]^{3\oplus}$ with ACl (A = Na or NBu_4).

Na salt: [61779-28-0].
Yellow salt. Mp 240° dec.

Tetrabutylammonium salt: Red salt. Mp 145°.

Bora, T. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 1815 (*synth, ir*)

$C_4H_{12}Cl_4O_2S_2Tc$ IC-004240

Tetrachlorobis(dimethyl sulfoxide)technetium(*IV*)

Tetrachlorobis[sulfinylbis[methane]-O]technetium. Technetium(IV) *chloride bis(dimethyl sulfoxide)*

[128955-36-2]

$TcCl_4(O{=}SMe_2)_2$

M 396.9

Synth. from $TcCl_4(PPh_3)_2$. Pale yellow solid; paramagnetic. Sol. MeCN; spar. sol. Et_2O.

Breikss, A.I. *et al*, *Inorg. Chim. Acta*, 1990, **170**, 75 (*synth, ir, pmr, ms*)

$C_4H_{12}Cl_4O_2Ti^{\ominus}$ IC-004241

Tetrachlorobis(ethanol)titanate(*III*)(1−), 11Cl

[94596-09-5]

$(EtOH)_2TiCl_4^{\ominus}$

M 281.8 (ion)

cis-Octahedral anion. Synth. by adding HCl to a soln of $TiCl_3$ in EtOH. (In abscence of HCl, Trichlorotris(ethanol)titanium(*III*), IC-005341 is formed).

Kuchmii, S.Ya. *et al*, *Koord. Khim.*, 1984, **10**, 1505; *CA*, **102**, 71612m (*synth, ir, uv-vis, esr*)

$C_4H_{12}Cl_4O_2Ti$ IC-004242

Tetrachlorobis(dimethyl ether)titanium(*IV*)

Tetrachlorobis[oxybis[methane]]titanium(IV), *11Cl. Titanium tetrachloride bis(dimethyl ether). Titanium*(IV) *chloride bis(dimethyl ether)*

[57965-48-7]

$(Me_2O)_2TiCl_4$

M 281.8

Formed as a mixt. of octahedral *cis* and *trans* isomers. Synth. by co-condensing $TiCl_4$ and Me_2O *in vacuo*.

[89253-92-9, 89253-93-0]

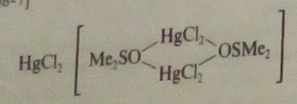
Valloton, M. *et al*, *Helv. Chim. Acta*, 1975, **58**, 2272 (*synth, uv-vis*)
Tan, L.K. *et al*, *Inorg. Chem.*, 1984, **23**, 1353 (*pmr*)

$C_4H_{12}Cl_6Hg_3O_2S_2$ IC-004243

Hexachlorobis(dimethyl sulfoxide)trimercury

Hexachlorobis[sulfinylbis[methane]]trimercury. Di-μ-chloro-μ$_3$-chlorotrichlorobis[sulfinylbis[methane]-O]trimercury. Mercury(II) *chloride dimethyl sulfoxide complex (3:2)*

[36248-68-7]



M 970.7

Tablets (EtOH or C_6H_6). Mp 123-125°.

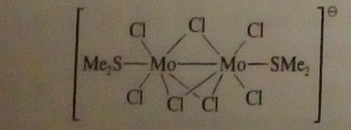
[12602-92-5, 55405-06-6]

Biscarini, P. *et al, J. Chem. Soc. A*, 1971, 1128 (*synth*)
Biscarini, P. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1003; 1974, 1846 (*ir, raman, cryst struct*)
Ramakrishnan, L. *et al, Indian J. Chem., Sect. A*, 1979, **18**, 287 (*Cl-35 nqr*)
Konovalov, L. *et al, J. Coord. Chem.*, 1986, **14**, 207 (*ir*)

$C_4H_{12}Cl_7Mo_2S_2^{\ominus}$ IC-004244

Tri(μ-chloro)tetrachlorobis(dimethyl sulfide) dimolybdate(*IV*)(1−)

Tri-μ-chlorotetrachlorobis[thiobis[methane]]dimolybdate(IV) *(1−), 11Cl*



M 564.3 (ion)

Distorted confacial bioctahedral framework, with a weak metal-metal interaction. The Mo atoms are antiferromagnetically coupled.

Ph_4P salt: [83779-65-1].
Triclinic cryst.

Boorman, P.M. *et al, J. Chem. Soc., Chem. Commun.*, 1982, 899 (*cryst struct, synth*)

$C_4H_{12}Cl_9NiP_4$ IC-004245

Tetrakis(methylphosphonous dichloride)nickel, 11Cl

Tetrakis[dichloro(methyl)phosphine]nickel(0)

[76404-15-4]

$Ni(PMeCl_2)_4$

M 526.3

First Ni(0) complex discovered after $Ni(CO)_4$ to be formed by direct synth. Air sensitive yellow solid. Sol. EtOH, pentane.

Quin, L.D., *J. Am. Chem. Soc.*, 1957, **79**, 3681 (*synth*)
Taylor, N.J., *J. Chem. Soc., Chem. Commun.*, 1985, 476 (*synth*)

$C_4H_{12}CoO_8S_4^{2\ominus}$ IC-004246

Tetrakis(methanesulfinato-*O*)cobaltate(*II*)(2−), 9Cl

$[Co[OS(O)Me]_4]^{2\ominus}$

M 375.3 (ion)

Prob. tetrahedral.

Bis-Ph_4P salt: [58904-97-5].
Blue-violet solid. Sol. EtOH, Me_2CO. Paramagnetic. Dec. at 190°

Lorenz, I.P. *et al, Inorg. Nucl. Chem. Lett.*, 1976, **12**, 141 (*synth, ir, uv, magnetism*)

$C_4H_{12}CoP_2S_4$ IC-004247

Bis(dimethyldithiophosphinato)cobalt(*II*)

Bis(dimethylphosphinodithioato-S,S′)cobalt(II), *9Cl*

[56199-77-0]

$[Co(S_2PMe_2)_2]_n$

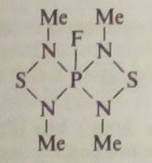
M 309.2

Struct. comprises infinite independent chains of tetrahedral Co atoms linked by alternating pairs of ligand bridges. Green cryst.

Cavell, R.G., *Inorg. Chem.*, 1972, **11**, 1759 (*synth, struct*)

$C_4H_{12}FN_4PS_2$ IC-004248

4-Fluoro-1,3,5,7-tetramethyl-2,6-dithia-1,3,5,7-tetraaza-4-phospha(4P^V)spiro[3.3]heptane, 8Cl



M 230.2

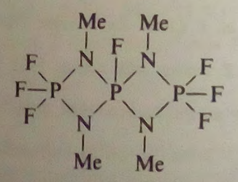
2,2,6,6-Tetraoxide: [21465-18-9].
$C_4H_{12}FN_4O_4PS_2$ M 294.2
Colourless hygroscopic cryst. (C_6H_6). V. sol. CH_2Cl_2, 1,2-dichloroethane; less sol. C_6H_6, CCl_4; insol. pet. ether. Mp 184-188° dec. (180-182°). Monomeric.

Becke-Goehring, M. *et al, Z. Anorg. Allg. Chem.*, 1969, **365**, 185; **371**, 88 (*synth, pmr, F-19 nmr, P-31 nmr*)

$C_4H_{12}F_7N_4P_3$ IC-004249

2,2,2,4,6,6,6-Pentafluoro-2,2,6,6-tetrahydro-1,3,5,7-tetramethyl-1,3,5,7-tetraaza-2,4,6-triphospha(4-P^V) spiro[3.3]heptane

[67485-36-3]



M 342.0

Colourless cryst. Mp 67-69°. Subl.$_{0.5}$ 40°.

Kubjacek, M. *et al, Monatsh. Chem.*, 1978, **109**, 587 (*synth, ms, ir*)

$C_4H_{12}FeO_4^{\ominus}$ IC-004250

Tetramethoxyferrate(*III*)(1−)

$[Fe(OMe)_4]^{\ominus}$ (T_d)

M 179.9 (ion)

Soln. species obsd. conductometrically in reaction of $FeCl_3$ with NaOMe. Sol. alcohols.

Na salt: [61385-33-9].
Not isol.

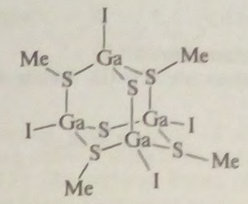
K salt: [15021-90-6].
Not isol.

Meerwein, H. *et al, Justus Liebigs Ann. Chem.*, 1929, **476**, 113 (*synth*)
Ludman, C.J. *et al, J. Chem. Soc. A*, 1966, 1816 (*synth*)
Jain, N.C. *et al, Proc. - Indian Acad. Sci., Sect. A*, 1976, **84**, 98.

$C_4H_{12}Ga_4I_4S_6$ IC-004251

Tetraiodotetrakis[μ-(methanethiolato)]di-μ-thioxotetragallium

[89788-68-1]



M 1039.0

'Adamantane'-like framework. Synth. from Ga_2I_4 and Me_2S_2. Colourless cryst. (Me_2S_2).

Boardman, A. *et al, Inorg. Chim. Acta*, 1984, **83**, L39 (*synth, cryst struct*)

$C_4H_{12}GeO_4$ IC-004252

Tetramethoxygermanium

Germanium(IV) *methoxide. Methanol, germanium*(4+) *salt (4:1)*

[992-91-6]

$Ge(OMe)_4$

M 196.7

Liq. d^{20} 1.325. Mp −18°. Bp 145°.

Bottei, R.S. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 415 (*pmr*)
Dube, G., *Z. Chem.*, 1969, **9**, 316 (*ms*)
Kaufman, J. *et al, Z. Naturforsch., A*, 1971, **26**, 1384 (*Ge-73 nmr*)
Skobeleva, S.E. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1973, **210**, 122 (*ir*)

$C_4H_{12}IN_2P$ IC-004253

Tetramethylphosphorodiamidous iodide, 11Cl

Tetramethylphosphoramidous iodide. Bis(dimethylamino) iodophosphine. Bis(dimethylamido)iodophosphorus(III)

[20502-38-9]

$(Me_2N)_2PI$

M 246.0

V. moisture-sensitive yellow liq. Bp_1 50°. Complexes with $AlCl_3$.

Mitel'man, I.E. *et al, Zh. Obshch. Khim.*, 1984, **54**, 1245; *J. Gen. Chem. USSR (Engl. Transl.)*, 1984, **54**, 1114 (*synth, props, P-31 nmr*)
Cypryk, M. *et al, Tetrahedron*, 1985, **41**, 2471 (*synth, ms, pmr, P-31 nmr*)

$C_4H_{12}IN_2PS$ IC-004254

Tetramethylphosphorodiamidothioic iodide, 11Cl

Iodobis(dimethylamido)thiophosphorus(V)

[93374-05-1]

$(Me_2N)_2P(S)I$

M 278.0

Liq. $Bp_{0.07}$ 75-76°.

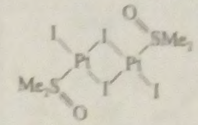
Mitel'man, I.E. *et al, Zh. Obshch. Khim.*, 1984, **54**, 1245; *J. Gen. Chem. USSR (Engl. Transl.)*, 1984, **54**, 1114 (*synth, P-31 nmr*)

$C_4H_{12}I_4O_2Pt_2S_2$ IC-004255

Bis(dimethyl sulfoxide)tetraiododiplatinum(*II*)

Tetraiodobis[sulfinylbis[methane]]diplatinum, 9Cl. Di-μ-iododiiodobis[sulfinylbis[methane]S]diplatinum, 10Cl

[39336-40-8]



M 1054.0

Structure assumed, not proven. Similar compds. exist for Cl, Br and other R_2SO ligands. Synth. from Me_2SO + $[PtI_4]^{2\ominus}$ or from Me_2SO + Dichlorobis(dimethyl sulfoxide)platinum(*II*), IC-004229 + $I^{\ominus}$. Red-brown solid. Sol. $CHCl_3$, DMSO.

Monomer: Platinum diiodide dimethylsulfoxide
$C_2H_6I_2OPtS$ M 527.0
Unknown.

[72557-01-8]

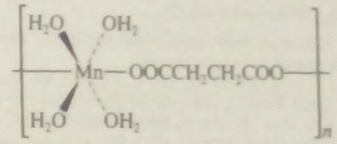
Kukushkin, Yu.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 595 (*synth*)
Kong, P.-C. *et al, Inorg. Chim. Acta*, 1979, **37**, L457 (*synth*)

$C_4H_{12}MnO_8$ IC-004256

Tetraaqua[butanedioato(2−)-*O*]manganese, 11Cl

Tetraaqua(μ-succinato)manganese(II)

[65629-64-3]



M 243.0

Polymeric chain struct. Cryst.

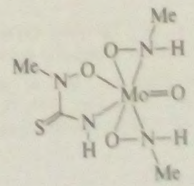
Gupta, M.P. *et al, Indian J. Phys., A*, 1977, **51**, 223 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 137 (*rev, bibl*)
Gupta, M.P. *et al, Z. Kristallogr.*, 1983, **163**, 155.

$C_4H_{12}MoN_4O_4S$ IC-004257

Bis(*N*-methylhydroxylamido-*N,O*)-(*N*-hydroxy-*N*-methylthioureato-*N,O*)-oxomolybdenum(*VI*)

Bis(N-hydroxymethanaminato-N,O)[N-hydroxy-N-methylthioureato(2−)-N′,O]oxomolybdenum, 10Cl

[74096-66-5]



M 308.1

7-Coordinate. Red cryst. Mp 140° dec.

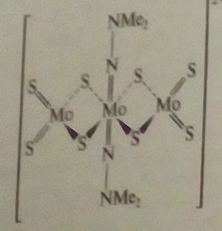
Wieghardt, K. *et al, Inorg. Chem.*, 1980, **19**, 2927 (*cryst struct, synth*)

IC-004258

$C_4H_{12}Mo_3N_4S_8^{2\oplus}$

Bis[1,1-dimethylhydrazinato(2−)-*N*²]tetra-μ-thioxotetrathioxotrimolybdate(2−), 11Cl

Bis[[bist(μ-sulfido)disulfidomo(ybdenum]-N,N-dimethylhydrazido]mo(ybdate(2−)



M 660.5 (ion)

Bis-Ph_4P salt: [80327-83-9].
Dark red-brown cryst.

Dilworth, J.R. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 365 (*cryst struct, synth*)

IC-004259

$C_4H_{12}NO_4Tc$

Tetramethylammonium pertechnetate

Tetramethylammonium technetate(VII)(*1*−)

[51292-85-4]

$(Me_4N)TcO_4$

M 237.0
Orthorhombic (CsCl struct.). Synth. from $[Me_4N]OH$ and $HTcO_4$. White solid (H_2O).

German, K.E. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1986, **287**, 650 (*synth, ir, powder struct*)
Kuzina, A.F. *et al*, *Zh. Neorg. Khim.*, 1987, **32**, 83; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1987, **32**, 44 (*thermal dec*)
German, K.E. *et al*, *Zh. Neorg. Khim.*, 1987, **32**, 1089; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1987, **32**, 667 (*synth, cryst struct, ir*)

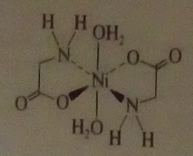
IC-004260

$C_4H_{12}N_2NiO_6$

Diaquabis(glycinato-*N,O*)nickel(*II*)

Bis(glycinato)diaquanickel(II). *Nickel glycinate*

[14215-54-4]



M 242.8
trans-Octahedral at Ni. Light blue cryst. Sol. H_2O. Paramagnetic; antiferromagnetic below 0.88K.

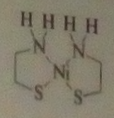
Stosick, A.J., *J. Am. Chem. Soc.*, 1945, **67**, 365 (*synth, cryst struct*)
Sen, D.N. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 211 (*synth, ir*)
Castellano, E.E. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 1303 (*cryst struct*)

IC-004261

$C_4H_{12}N_2NiS_2$

Bis(2-aminoethanethiolato-*N,S*)nickel(*II*)

[53496-00-7]



M 210.9
Square planar struct. Light green cryst. Sol. org. solvs. Reacts at S with metal or organic halides.

Busch, D.H. *et al*, *Inorg. Chem.*, 1962, **1**, 872 (*synth*)

IC-004262

$C_4H_{12}N_2O_4Zn$

Bis(acetato-*O*)diamminezinc(*II*)

Diamminezinc bisacetate. Zinc(II) *acetate diammine*

[15633-92-8]

$(H_3N)_2Zn(OAc)_2$

M 217.5
Cryst.

[32965-77-8]

Spacu, G. *et al*, *Z. Anorg. Allg. Chem.*, 1936, **227**, 129.
Grigor'ev, A.L., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 1358 (*ir*)
Bernard, M.A. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 2110 (*heat of formn*)
Grigor'ev, A.L. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1971, **12**, 240 (*ir*)
Mikler, H. *et al*, *Monatsh. Chem.*, 1974, **105**, 742 (*synth, struct*)

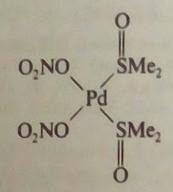
IC-004263

$C_4H_{12}N_2O_8PdS_2$

Bis(dimethylsulfoxide)dinitratopalladium(*II*)

Bis(nitrato-O)bis[sulfinylbis[methane]-S]palladium, 9CI

[69417-26-1]



cis-form

M 386.6
Square planar.

cis-form [19995-58-5]
Synth. from $Pd(NO_3)_2$ and DMSO. Orange-yellow cryst. ($MeNO_2$). Mp 143-145°.

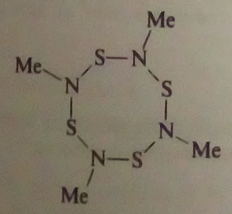
Langs, D.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 1080 (*synth, cryst struct*)

IC-004264

$C_4H_{12}N_4S_4$

2,4,6,8-Tetramethyl-1,3,5,7,2,4,6,8-tetrathiatetrazocine

[28924-12-1]



M 244.4
Interatomic distances: S—N 167.7, C—N 147.9 pm; ring has crown conformn. Formed from $MeNH_2 + SCl_2$ together with polymeric and other products. Colourless needles. Sol. hexane, MeOH. Bp 126-126.5°. Dec. at 190°.

Stone, B.D. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 3580 (*synth, ir, raman*)
Macdonald, A.L. *et al*, *Can. J. Chem.*, 1973, **51**, 2504 (*cryst struct*)

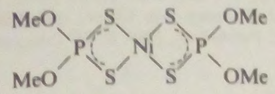
IC-004265

$C_4H_{12}NiO_4P_2S_4$

Bis(*O,O*-dimethyldithiophosphato)nickel(*II*)

Bis(O,O-*dimethylphosphorodithioato-S,S′)nickel, 11Cl*

[15844-04-9]



M 373.0
Square planar nickel. Used in synth. of pressure sensitive colour copying sheets. Purple cryst. Sol. Me_2CO, most org. solvs. H_2O. Diamagnetic. Forms adducts with various Lewis bases; phosphines cause reduction.

Bis-Py complex:
$C_{14}H_{22}N_2NiO_4P_2S_4$ M 531.2
Green cryst.

Phen complex: [29946-07-4].
$C_{16}H_{20}N_2NiO_4P_2S_4$ M 553.2
Bright green needles (Me_2CO/EtOH). Sol. Me_2CO. Contains *cis*-octahedral Ni.

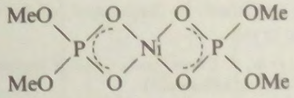
Kastalski, V. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 909 (*cryst struct*)
Sketty, P.S. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 3964 (*complexes cryst struct*)
Myers, K. *et al*, *J. Phys. Chem.*, 1973, **77**, 280 (*pe*)
Tomlinson, A.A.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 1420 (*synth, complex, uv-vis*)
Rudzinski, W. *et al*, *Inorg. Chem.*, 1977, **16**, 1206 (*ir*)
Faijyaz, M.V. *et al*, *Aust. J. Chem.*, 1978, **31**, 1439.
Black, L.F. *et al*, *Inorg. Chim. Acta*, 1978, **30**, L327 (*synth, complexes*)
Japan. Pat., 80 53 593, (1980); *CA*, **93**, 213421 (*use*)
Mukherjee, R.N. *et al*, *Thermochim. Acta*, 1982, **57**, 387 (*complexes*)

IC-004266

$C_4H_{12}NiO_8P_2$

Bis(dimethylphosphato-*O′,O″*)nickel(*II*)

[62532-30-3]



M 308.7
Hygroscopic yellow solid. $\mu_{eff} = 3.21\mu_B$. Forms 2:1 adducts with Lewis bases, prob. 6-coord. monomers.

Dihydrate: [62301-14-8]. *Diaquabis(dimethylphosphato) nickel*
$C_4H_{16}NiO_{10}P_2$ M 344.8
Green solid. $\mu_{eff} = 3.12\mu_B$.

Bis-Py complex: [62301-10-4]. *Bis(dimethylphosphato) bis(pyridine)nickel*
$C_{14}H_{22}N_2NiO_8P_2$ M 466.9
Green solid. $\mu_{eff} = 3.30\mu_B$.

Bis(isoquinoline) complex: [62301-13-7].
$C_{22}H_{26}N_2NiO_8P_2$ M 567.0
Green solid. $\mu_{eff} = 3.30\mu_B$.

Bis(γ-picoline) complex: [62301-11-5].
$C_{16}H_{26}N_2NiO_8P_2$ M 495.0
$\mu_{eff} = 3.30\mu_B$.

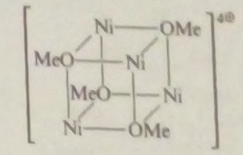
Gutman, V. *et al*, *Monatsh. Chem.*, 1968, **99**, 1452 (*synth, magnetism, ir*)
Paul, R.C. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **13**, 21 (*synth, adducts, uv-vis*)

IC-004267

$C_4H_{12}Ni_4O_4^{4\oplus}$

Tetramethoxytetranickel(*II*)(4+)

Tetramethoxotetranickel(II)(4+)



M 358.8 (ion)
Cluster found in various polynuclear Ni complexes. Tends to show ferromagnetic coupling between Ni ions.

Tetrakis-acetylacetonate, tetra-MeOH complex: see *Tetrakis(methanol)tetra-μ₃-methoxytetrakis(2,4-pentanedionato-O,O′)tetranickel*(II), *IC-012246*
Tetrakis(2-hydroxybenzaldehydate), tetra-MeOH complex: see *Tetrakis(2-hydroxybenzaldehydato-O¹,O²) tetrakis(methanol)tetra-μ₃-methoxytetranickel*(II), *IC-013495*

Andrew, J.E. *et al*, *J. Chem. Soc. A*, 1969, 1456 (*synth, magnetism*)
Bertrand, J.A. *et al*, *Inorg. Chem.*, 1971, **10**, 240 (*synth, magnetism*)
Ginsberg, A.P., *Inorg. Chim. Acta Rev.*, 1971, **5**, 45 (*rev*)
Gladfelter, W.L. *et al*, *Inorg. Chem.*, 1981, **20**, 2390 (*synth, magnetism*)

IC-004268

$C_4H_{12}O_4Si$

Tetramethoxysilane

Silicic acid tetramethyl ester, 9CI. Methyl orthosilicate. Tetramethyl silicate

[681-84-5]

$Si(OMe)_4$ (T_d)

M 152.2
Cocatalyst with CsF for Michael additions. Liq. d_4^{22} 1.03. Mp 4-5°. Bp 120-121°, Bp_{34} 42.5°.

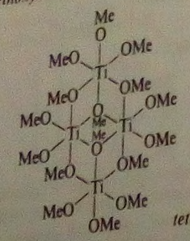
▷ Highly toxic, v. irritating to eyes. TLV 30. VV9800000.

Emblem, H.G. *et al*, *Chem. Ind.* (*London*), 1966, 1296 (*synth*)
Nagy, J. *et al*, *Acta Chim. Acad. Sci. Hung.*, 1967, **52**, 319.
Sobolevskii, M.V. *et al*, *Khim. Promst.* (*Moscow*), 1971, **47**, 888; *CA*, **76**, 58895 (*synth*)
Ypenburg, Y.W. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1972, **391**, 1245 (*ir, raman*)
Engelhardt, G. *et al*, *Org. Magn. Reson.*, 1973, **5**, 561 (*cmr, Si-29 nmr*)
Boonstra, L.H. *et al*, *J. Mol. Struct.*, 1975, **28**, 129 (*struct*)
Shih, P.T.K. *et al*, *Mater. Sci. Eng.*, 1975, **20**, 145 (*raman*)
van den Berghe, E.V. *et al*, *J. Organomet. Chem.*, 1976, **122**, 329 (*Si-29 nmr, synth, pmr*)
Lischke, G. *et al*, *Z. Chem.*, 1986, **26**, 178.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 501.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2389.

$C_4H_{12}O_4Ti$ IC-004269

Titanium(*IV*) methoxide ($Ti(OMe)_4$)

Tetramethoxytitanium. Titanium tetramethoxide



tetramer

M 172.0

Oligomeric. Synth. either by reaction of $TiCl_4$, MeOH and NH_3 or from $Ti[OCH(CH_3)_2]_4$ and MeOH. Used in olefin and ester polym. catalysts and in the formation of TiO_2 thin-film capacitors. Liq., readily hydrol.

Trimer: [12563-47-2].
$C_{12}H_{36}O_{12}Ti_3$ M 516.0
Yellow liq. Mp 209-210°. Only indirect soln. evidence exists for this formulation.

Tetramer: Di-μ_3-methoxytetra-μ-methoxydecamethoxytetratitanium(IV)
$C_{16}H_{40}O_{16}Ti_4$ M 688.0
Existence confirmed by X-ray diffraction. Ti in octahedral environment.

Dunn, P., *Austr. J. Appl. Sci.*, 1959, **10**, 458 (*synth*)
Deluzarche, A., *Ann. Chim. (Paris)*, 1961, **6**, 661 (*synth, trimer*)
Brini-Fritz, M. *et al*, *Bull. Soc. Chim. Fr.*, 1961, 535 (*ir, trimer*)
East Ger. Pat., 43, 616, (1965); *CA*, **64**, 19830d (*use*)
Weingarten, H. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 724 (*synth, pmr*)
Sianesi, D. *et al*, *Makromol. Chem.*, 1965, **81**, 264 (*use*)
Wright, D.A. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 1107 (*cryst struct, tetramer*)
Gut, R. *et al*, *Helv. Chim. Acta*, 1971, **54**, 593 (*props, trimer*)

$C_4H_{12}O_4Zn^{2\ominus}$ IC-004270

Tetramethoxyzincate(2 –)

$[Zn(OMe)_4]^{2\ominus}$

M 189.5 (ion)

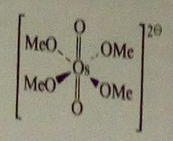
Di-Na salt: [52827-32-4].
Synth. from $ZnCl_2$ and NaOMe in MeOH. Solid. Monomeric in MeOH.

Shiner, V.J. *et al*, *Inorg. Chem.*, 1975, **14**, 157 (*synth*)

$C_4H_{12}O_6Os^{2\ominus}$ IC-004271

Tetramethoxydioxoosmate(*VI*)(2 –)

[120169-51-9]



M 346.3 (ion)

Di-K salt: [37549-62-5].
Synth. by adding MeOH soln. of KOH to OsO_4 in MeOH. Synthetic reagent, e.g. in carboxylation reactions at OMe. Brown solid.

Bis-Me_4N salt: [125081-64-3].
Synth. by adding MeOH soln. of $[NMe_4]OH$ to OsO_4 in MeOH.

Bis-tetrabutylammonium salt: [125115-45-9].
Criegee, R., *Justus Liebigs Ann. Chem.*, 1936, **75**, 522 (*synth*)
Griffith, W.P., *J. Chem. Soc.*, 1964, 245 (*ir*)
Kharitonov, Y.Y. *et al*, *Zh. Neorg. Khim.*, 1967, **12**, 1592 (*ir*)
Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1449 (*ir*)
Nielsen, A.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1501 (*use*)
Sartori, C. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **565**, 23 (*use*)
Arnold, J. *et al*, *Polyhedron*, 1989, **8**, 597 (*use, synth*)

$C_4H_{12}O_6PdS_2$ IC-004272

Bis(dimethylsulfoxide)sulfatopalladium(*II*)

[Sulfato(2 –)]bis[sulfinylbis[methane]]palladium

$(Me_2SO)_2Pd(SO_4)$

M 358.7

Prob. contains chelating sulfato groups. Prepd. by addition of 2,2-dimethoxypropane to a filtered soln. of $PdSO_4.2H_2O$ in DMSO. Yellow solid. V. hygroscopic.

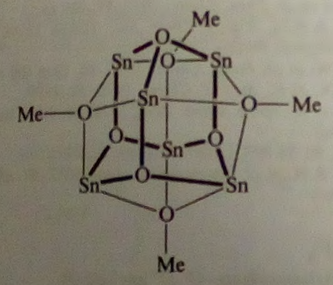
Eskenazi, R. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 521 (*synth, ir*)

$C_4H_{12}O_8Sn_6$ IC-004273

Tetra-μ_3-methoxytetra-μ_3-oxohexatin, 9CI

Tetramethoxytetraoxyhexastannane

[67450-12-8]



M 900.3

Has an adamantane-like skeleton with overall ~ D_{2d} symmetry. Intermed. in the hydrol. of $Sn(OMe)_2$. Monoclinic cryst.

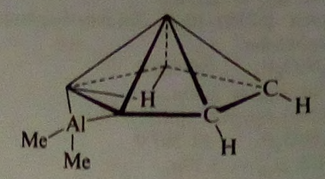
Harrison, P.G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 112 (*synth, cryst struct, mössbauer*)

$C_4H_{13}AlB_4$ IC-004274

[(2,6-η)-Heptahydro-4,5-dicarbahexaborato(1 –)] dimethylaluminium

μ-Dimethylaluminium-2,3-η-dicarbahexaborane

[55663-16-6]



M 131.3

nido-Tentative struct. shown. Extremely unstable in soln. or liq. phase, characterised by ms. Sl. volatile liq.

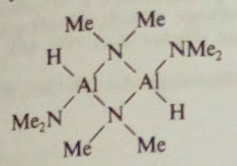
Magee, C.P. *et al*, *J. Organomet. Chem.*, 1975, **86**, 159 (*synth*)

$C_4H_{13}AlN_2$ IC-004275

Bis(dimethylamido)hydroaluminium

Bis(dimethylamino)alane

[2826-17-7]



Dimer

M 116.1

Dimeric. Reagent for hydrometallation of alkenes. Analogous diethyl and diisopropyl-amino derivs. also descr.

Dimer: [88764-40-3]. *Dihydrobis[μ-(N-methylmethanaminato)]bis(N-methylmethanaminato) dialuminium, 11CI*
$C_8H_{26}Al_2N_4$ M 232.2
Synth. from Me_3NAlH_3 and Me_2NH. Colourless air and moisture sensitive solid (by subl.). Sol. Et_2O, C_6H_6. Mp 63-65°. $Subl._{0.001}$ 35-50°.

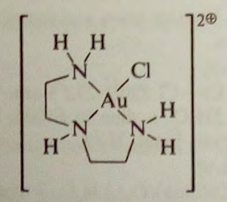
Wiberg, E. *et al*, *Z. Naturforsch., B*, 1955, **10**, 234 (*synth*)
Ruff, J.K. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2835 (*synth*)
Kovar, R.A. *et al*, *Inorg. Chem.*, 1971, **10**, 893 (*synth, pmr*)
Keller, P.C., *J. Am. Chem. Soc.*, 1974, **96**, 3073 (*reactions*)
Ashby, E.C. *et al*, *J. Org. Chem.*, 1979, **44**, 4364 (*use*)
Takahashi, Y. *et al*, *J. Mater. Sci.*, 1981, **16**, 1217 (*synth*)
Ouzounis, K. *et al*, *Z. Anorg. Allg. Chem.*, 1983, **504**, 67 (*cryst struct*)

$C_4H_{13}AuClN_3^{2\oplus}$ IC-004276

Chloro(diethylenetriamine)gold(*III*)(2+)

[N-(*2-Aminoethyl*)-*1,2-ethanediamine*-N,N′,N″] *chlorogold*(2+), *10CI, 9CI*. [*Bis*(2-*aminoethyl*)*amine*] *chlorogold*(III)(2+)

[61168-75-0]



M 335.5 (ion)

Distorted square planar geometry. Interatomic distances: Au—Cl 227.3, Au—N 205, 198, 197 pm; angles: ClAuN 176.4, 94.9, 93.8°. Behaves as acid in aq. soln. forming conj. base.

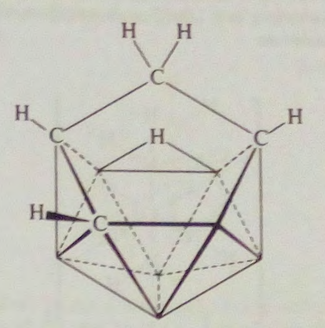
Dichloride: [61168-73-8].
$C_4H_{13}AuCl_3N_3$ M 406.4
Stable yellow cryst. Sol. H_2O.
Chloride perchlorate: [73432-42-5].
Monoclinic cryst.
▷ Potentially explosive.

Baddely, W.H. *et al*, *Inorg. Chem.*, 1963, **2**, 921 (*synth, uv-vis*)
Nardin, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 220 (*synth, cryst struct*)

$C_4H_{13}B_7$ IC-004277

6,9-μ-Methylene-5,6,9-tricarbadecaborane(11), 12CI

[114901-03-0]



M 136.8

arachno-. Sol. hexane, $CHCl_3$.

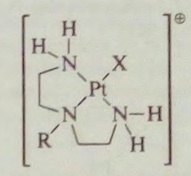
Stibr, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1106 (*synth, pmr, B-11 nmr, cmr, ms*)

$C_4H_{13}BrN_3Pt^{\oplus}$ IC-004278

Bromo(diethylenetriamine)platinum(*II*), 8CI

Bromo(1,4,7-triazaheptane)platinum(II). [N-(*2-Aminoethyl*)-*1,2-ethanediamine*]*bromoplatinum*(1+), *9CI*

[15522-24-4]



R = H, X = Br

M 378.1 (ion)

Many kinetic studies of substitutions, especially with DNA components, to investigate antitumour behaviour.

▷ May provoke an allergic response.

Bromide: [15633-95-1].
$C_4H_{13}Br_2N_3Pt$ M 458.0
Yellow cryst.

Tetrabromoplatinate(II) (*2:1*): [70212-03-2].
$C_8H_{26}Br_6N_6Pt_3$ M 1270.9
Cryst.

Watt, G.W. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 6382 (*synth*)
Cleare, M.J. *et al*, *Bioinorg. Chem.*, 1973, **2**, 187 (*antitumour*)
Melanson, R. *et al*, *Can. J. Chem.*, 1975, **53**, 1139 (*struct*)
Cleare, M.J. *et al*, *Clin. Allergy*, 1976, **6**, 183 (*allergy*)
Melanson, R. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 736 (*synth, struct*)

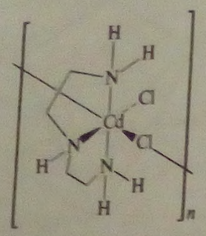
IC-004279

$C_4H_{13}CdCl_2N_3$

Dichloro(diethylenetriamine)cadmium

[N-2-(Aminoethyl)-1,2-ethanediamine-N,N',N'']dichlorocadmium, 9CI. *[Bis(2-aminoethyl)amine]dichlorocadmium*

[76404-59-6]



M 286.4

Polymeric chain struct. Cryst. (aq. MeOH). Sol. H_2O, DMSO; insol. MeOH, EtOH, $Me_2CO/CHCl_3$.

[37450-69-4]

Cova, G. *et al*, *Inorg. Chim. Acta*, 1972, **6**, 343 (*synth, props, ir*)
Cannus, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 2090 (*cryst struct, synth*)

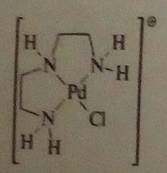
IC-004280

$C_4H_{13}ClN_3Pd^{\oplus}$

Chloro(diethylenetriamine)palladium(*II*)(1+)

[N-(2-Aminoethyl)-1,2-ethanediamine-N,N',N'']chloropalladium(1+), 9CI

[17549-31-4]



M 245.0 (ion)

Chloride: [23041-96-5].
$C_4H_{13}Cl_2N_3Pd$ M 280.4
Prepd. from $PdCl_2$ with diethylenetriamine.3HCl.
Yellow cryst. (aq. EtOH).

[84992-76-7]

Basolo, F. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 4200; 1966, **88**, 2944 (*synth*)
Watt, G.W. *et al*, *Spectrochim. Acta, Part A*, 1964, **20**, 1053 (*ir*)
Chin, P.-K.C. *et al*, *Inorg. Chem.*, 1976, **15**, 982 (*cmr*)
Games, D.E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1994 (*ms*)

IC-004281

$C_4H_{13}ClN_3Pt^{\oplus}$

Chloro(diethylenetriamine)platinum(*II*), 8CI

Chloro(1,4,7-triazaheptane)platinum(II). [N-(*2-Aminoethyl*)-*1,2-ethanediamine]chloroplatinum(1+), 9CI*

[15522-23-3]

As Bromo(diethylenetriamine)platinum(*II*), IC-004278 with

R = H, X = Cl

M 333.7 (ion)

Many investigations on possible antitumour properties. Kinetics of substitutions studied, particularly with DNA components.

▷ May induce allergic response. TP2275640.

Chloride: [14215-58-8].
$C_4H_{13}Cl_2N_3Pt$ M 369.1
Yellow cryst. Sol. H_2O.
▷ TP2275660.

Watt, G.W. *et al*, *Inorg. Chem.*, 1968, **7**, 335 (*synth, ir*)
Cleare, M.J. *et al*, *Bioinorg. Chem.*, 1973, **2**, 187 (*antitumour*)
Cleare, M.J. *et al*, *Clin. Allergy*, 1976, **6**, 183 (*allergy*)
Butour, J.L. *et al*, *Biochim. Biophys. Acta*, 1981, **653**, 305 (*DNA reaction*)
Britten, J.F. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2148 (*cryst struct*)

IC-004282

$C_4H_{13}Cl_2CrN_3$

Dichloro(diethylenetriamine)chromium(*II*)

$CrCl_2(H_2NCH_2CH_2NHCH_2CH_2NH_2)$

M 226.0

Presumably polymeric. Blue air-sensitive solid. μ_{eff} = $4.38\mu_B$ (300K); $3.39\mu_B$ (90K). Corresp. bromide and iodide alsoreported.

Earnshaw, A. *et al*, *J. Chem. Soc. A*, 1969, 2276 (*synth, props*)
Crouse, K. *et al*, *Inorg. Chim. Acta*, 1985, **99**, 199 (*synth, reactions*)

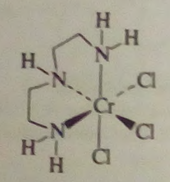
IC-004283

$C_4H_{13}Cl_3CrN_3$

Trichloro(diethylenetriamine)chromium(*III*), 8CI

[N-(2-Aminoethyl)-1,2-ethanediamine-N,N',N'']trichlorochromium, 9CI. Trichloro(1,5-diamino-3-azapentane)chromium(III)

[15633-96-2]



fac-form

M 261.5

Hydrol. of both isomers gives various octahedral aqua and hydroxo derivs.

fac-form [15025-05-5]

Cr—N_a, 209, Cr—Cl 230.3-232.5 pm. Synth. from $[Cr(urea)_6]Cl_3.3H_2O$ + dien in EtOH, followed by conc. HCl. Green cryst. Insol. H_2O.

mer-form [15244-12-9]

Synth. from $[Cr(dien)(O_2)_2].H_2O$ + conc. aq. HCl. Purple solid. Insol. cold H_2O. λ_{max} 420sh, 530, 638 nm.

[15025-05-5]

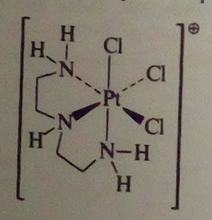
House, D.A. *et al*, *Inorg. Chem.*, 1966, **5**, 840 (*synth, uv-vis*)
Fowlie, A.D. *et al*, *J. Chem. Soc. A*, 1970, 803 (*cryst struct, uv-vis, fac-form*)
Garner, C.S. *et al*, *Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 807 (*rev*)

IC-004284

$C_4H_{13}Cl_3N_3Pt^{\oplus}$

Trichloro(diethylenetriamine)platinum(*IV*)

1,4,7-Triazaheptanetrichloroplatinum(IV). [N-(*2-Aminoethyl*)-*1,2-ethanediamine]trichloroplatinum(1+), 9CI*



M 404.6 (ion)

Chloride has *fac*-configuration. Other salts poorly characterised.

Chloride: [76822-17-8].
$C_4H_{13}Cl_4N_3Pt$ M 440.0
Yellow cryst. + $1H_2O$.

[86161-20-8]

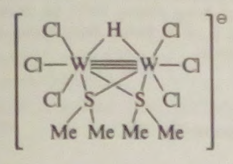
Britten, J.F. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 2958 (*cryst struct*)

IC-004285

$C_4H_{13}Cl_6S_2W_2^{\ominus}$

Hexachlorobis(μ-dimethyl sulfide)(μ-hydrido) ditungstate(*III*)(1−)

Hexachloro-μ-hydrobis[μ-thiobis[methane]]ditungstate(1−), 11CI



M 705.6 (ion)

W—W triple bond, 241.9 pm. Diamagnetic.

Ph_4P salt: [97295-68-6].
Purple-red cryst. + $2CH_2Cl_2$ (CH_2Cl_2/hexane).

Boorman, P.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1981, 1286 (*cryst struct, ir, nmr*)
Boorman, P.M. *et al*, *Inorg. Chem.*, 1985, **24**, 2989 (*ir, nmr, cryst struct*)

IC-004286

$C_4H_{13}IN_3Pt^{\oplus}$

Diethylenetriamine(iodo)platinum(*II*), 8CI

[N-(2-Aminoethyl)-1,2-ethanediamine]iodoplatinum(1+), 9CI. Iodo(1,4,7-triazaheptane)platinum(1+)

[22418-33-3]

As Bromo(diethylenetriamine)platinum(*II*), IC-004278 with

R = H, X = I

M 425.1 (ion)

A *cis*-N can be methylated. Kinetics of substitutions studied.

▷ May induce allergic response.

Iodide: [18509-61-0].
$C_4H_{13}I_2N_3Pt$ M 552.0
Yellow cryst. Sol. H_2O.
$[Pt(dien)I_3]^{\oplus}$ double salt, diiodide: [87890-56-0].
$C_8H_{26}I_6N_6Pt_2$ M 1357.9
Bronze cryst. Stacked columnar struct.

[87517-20-2]

Watt, G.W. *et al*, *Inorg. Chem.*, 1968, **7**, 335 (*synth*)
Watt, G.W. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 6382 (*ir*)
Cleare, M.J. *et al*, *Clin. Allergy*, 1976, **6**, 183 (*allergy*)
Mochida, I. *et al*, *Inorg. Chem.*, 1983, **22**, 1834.
Clark, R.J.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 1583 (*synth, raman, uv-vis, cryst struct*)

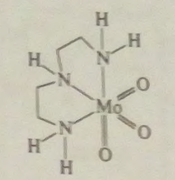
IC-004287

$C_4H_{13}MoN_3O_3$

(Diethylenetriamine)trioxomolybdenum(*VI*), 8CI

[N-(2-Aminoethyl)-1,2-ethanediamine]trioxomolybdenum(VI), *10CI, 9CI. Trioxo(diethylenetriamine)molybdenum*(VI)

[19478-36-5]



M 247.1

fac-Octahedral. Synth. from MoO_3 + the amine. Catalyses oxidation of ketones by H_2O_2. Added to molten steel to increase N content. White cryst. (aq. EtOH). Hydrol. in soln. to give $[MoO_4]^{2\ominus}$. V. sol. H_2O; insol. org. solvs. Ir ν_{MoO} 876s,br, 825vs,br cm^{-1} (nujol).

Marzluff, W.F., *Inorg. Chem.*, 1964, **3**, 395 (*synth*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1964, **3**, 397 (*cryst struct*)
Schmidtke, H.H. *et al*, *Inorg. Chim. Acta*, 1968, **2**, 357 (*ir*)
Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1968, 400 (*ir, raman*)
Taylor, R.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 24 (*ir, raman, props*)

IC-004288

$C_4H_{13}N_2OP$

N,N,N',N'-Tetramethylphosphonic diamide, 9CI

Phosphonic bis(dimethylamide). N,N,N',N'-*Tetramethylphosphorodiamidous acid. Hydrobis(dimethylamido)oxophosphorus*(V). *Hydroxybis(dimethylamido)phosphorus*(III)

[5843-26-5]

$$(Me_2N)_2P(O)H \rightleftharpoons (Me_2N)_2POH$$

M 136.1

Tautomeric. Liq. $Bp_{1.3}$ 56°. $n_D^{24.5}$ 1.4515.

Zwierzak, A., *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 609 (*synth, ir*)
Gallagher, M.J. *et al*, *J. Chem. Soc. C*, 1966, 2176 (*synth, ir, pmr*)
Wolf, R. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 1641 (*ir*)
Corey, E.J. *et al*, *J. Org. Chem.*, 1969, **34**, 3053 (*synth, ir, pmr*)
Burgada, R. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 192 (*synth, ir, pmr*)
Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **461**, 187 (*P-31 nmr*)

IC-004289

$C_4H_{13}N_4O_3Pt^{\oplus}$

Diethylenetriamine(nitrato)platinum(*II*)(1+)

[N-(2-Aminoethyl)-1,2-ethanediamine](nitrato-O) platinum(1+), 11CI. Nitrato(1,4,7-triazaheptane)platinum(II)

As Bromo(diethylenetriamine)platinum(*II*), IC-004278 with

R = H, X = ONO_2

M 360.2 (ion)

$NO_3^{\ominus}$ is *O*-bonded to Pt. $NO_3^{\ominus}$ is fastest leaving group in $[Pt(dien)X]^{\oplus}$ complexes.

Nitrate: [83857-38-9].
$C_4H_{13}N_5O_6Pt$ M 422.2
Colourless cryst. Sol. H_2O.

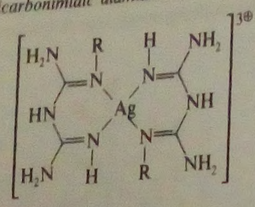
Basolo, F. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 4200 (*synth*)
Gray, H.B. *et al*, *Inorg. Chem.*, 1962, **1**, 481.
Britten, J.F. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2148 (*synth, raman, cryst struct*)

IC-004290

$C_4H_{14}AgN_{10}^{3\oplus}$

Bis(biguanidine)silver(*III*)(3+)

Bis(imidodicarbonimidic diamide-N″,N‴)silver(III)(3+), *9CI*



R = H

M 310.0 (ion)

Square planar at Ag.

Sulfate (2:3): [24899-83-0].
Yellow-brown soft cryst. Sol. H_2O; insol. org. solvs.

Trinitrate: [24968-35-2].
Yellow cryst. Sol. H_2O; insol. org. solvs.

Sen, D., *J. Chem. Soc.*, 1969, 1304 (*synth, magnetism*)
Swartz, W.E. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1974, **4**, 351 (*pe*)

IC-004291

$C_4H_{14}AlCl_3N_2$

Trichlorobis(dimethylamine)aluminium

Aluminium(III) *chloride bis(dimethylamine). Trichlorobis*(N-*methylmethanamine)aluminium, 10CI*

[65595-59-7]

$AlCl_3(NHMe_2)_2$

M 223.5

Monomeric trigonal bipyramidal Al with axial NMe_2H. Synth. from $AlCl_3$ and Me_2NH in C_6H_6 or Et_2O. Colourless air- and moisture-sensitive cryst. (by subl.). Mp 112-113°. $Subl._{0.01}$ 45°. Similar compds. also descr.

Beattie, I.R. *et al*, *J. Chem. Soc. A*, 1969, 2535 (*analogues*)
Ahmed, A. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **434**, 207 (*synth, cryst struct*)
Lobkovskii, E.B. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1978, **19**, 908 (*cryst struct*)

IC-004292

$C_4H_{14}BN$

(*tert*-Butylamine)trihydroboron

Trihydro(2-*methyl*-2-*propanamine*)*boron, 10CI. 2-Methyl*-2-*propanamine compd. with borane(1:1), 9CI.* tert-*Butylamine compd. with borane, 8CI. Borane* tert-*butylamine*

[7337-45-3]

$(H_3C)_3CNH_2{-}BH_3$

M 86.9

Used in photographic colour development. Water-soluble borane reducing agent for organic and inorganic compds. Comly. produced. Powder. Mp 98-100° dec., Mp 96°. Dipole moment 4.64D.

▷ Severe poison. EO3900000.

Nöth, H. *et al*, *Chem. Ber.*, 1960, **93**, 928; 1964, **97**, 110 (*synth*)
Purser, J.M. *et al*, *Inorg. Chem.*, 1968, **7**, 2156 (*nmr*)
Lane, C.F., *Aldrichimica Acta*, 1973, **6**, 51 (*rev*)
Compr. Org. Chem., Pergamon, Oxford, 1979, **3**, 695 (*rev*)

IC-004293

$C_4H_{14}BN$

(Diethylamine)trihydroboron

(N-Ethylethanamine)trihydroboron, 10CI. N-Ethylethanamine, compd. with borane(1:1), 9CI. Diethylamine compd. with borane(1:1), 8CI. Borane diethylamine

[2670-68-0]

$Et_2NH{-}BH_3$

M 86.9

Reducing agent in electrodeless coating procedures. Liq.

Laurent, J.P. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1966, **263**, 965 (*mord*)
Kovar, R.A. *et al*, *Inorg. Chem.*, 1971, **10**, 900; 1975, **14**, 2239 (*synth*)
Frick, W., *Oberflaechentechnik*, 1973, **50**, 450; *CA*, **80**, 43394a.
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*synth, ir, nmr*)
Ryschkewitsch, G.E. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1975, **5**, 123 (*synth*)

IC-004294

$C_4H_{14}B_2$

1,1-Diethyldiborane(6), 10CI

[62133-33-9]

As Methyldiborane(6), IC-002628 with

$R^1 = R^2 = Et$

M 83.7

Unstable with respect to disproportionation; sensitive to air and moisture. Sol. ethers, hydrocarbons.

Wrackmeyer, B., *J. Organomet. Chem.*, 1976, **117**, 313 (*nmr*)
Kuimova, M.E. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1979, 314; *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 288 (*nmr*)
Contreras, R. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1236.

IC-004295

$C_4H_{14}ClO_5V$

Chlorobis(methanol)bis(methoxy)oxovanadium(*V*), 11CI

[83762-11-2]

$VOCl(OMe)_2(MeOH)_2$

M 228.5

Octahedral. Synth. from $VOCl_3$ and MeOH in MeCN or CCl_4.

Konovalova, A.A. *et al*, *Koord. Khim.*, 1982, **8**, 1211; *CA*, **98**, 45771s (*synth, V-51 nmr*)

IC-004296

$C_4H_{14}Cl_2FeN_2$

Dichlorobis(ethylamine)iron(*II*)

Iron(II) *chloride bis(ethylamine)*

$FeCl_2(NH_2Et)_2$ (C_{2v})

M 216.9

Synth. from $FeCl_2$ or $FeCl_3$ + $EtNH_2$. White cryst. μ_{eff} = 5.3μ_B.

McGregor, W.R. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1027 (*synth, magnetism, ir*)

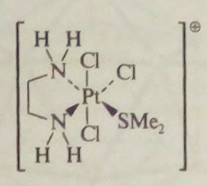
IC-004297

$C_4H_{14}Cl_3N_2PtS^{\oplus}$

Trichloro(dimethylsulfide)ethylenediamineplatinum(*IV*)

Trichloro(1,2-*ethanediamine*-N,N′)[*thiobis*(*methane*)]*platinum*(1+), *9CI*

[60927-58-4]



M 423.6 (ion)

Unusual example of Pt(*IV*) with S donor ligand. Synth. from chlorination of $[PtCl(en)(SMe_2)]^{\oplus}$. SEt_2 analogue also known.

Chloride: [58103-83-6].
$C_4H_{14}Cl_4N_2PtS$ M 459.1
White (?) cryst. Sol. H_2O.

Kukushkin, Yu.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 1728.

IC-004298

$C_4H_{14}Cl_4O_2P_2Ti$

Tetrachlorobis(dimethylphosphine oxide-*O*)titanium(*IV*), 11CI

Titanium(IV) *chloride bis(dimethylphosphine oxide)*

$(Me_2HPO)_2TiCl_4$

M 345.7

Octahedral.

cis-form [93556-83-3]
Synth. from $TiCl_4$ + Me_2HPO.

Muratova, A.A. *et al*, *Zh. Obshch. Khim.*, 1984, **54**, 1745; *CA*, **102**, 6730j (*synth, ir*)

IC-004299

$C_4H_{14}CoO_8$

Bis(acetato-*O*)tetraaquacobalt, 10CI

Diacetatotetraaquacobalt(II). *Cobaltous acetate tetrahydrate*

[19621-58-0]

$Co(OAc)_2(OH_2)_4$

M 249.0

trans-Octahedral with Co—OH_2 211, 206, Co—O 212 pm. Isomorphous with corresp. nickel acetate complex. Pinkish red cryst. Loses H_2O at 140°.

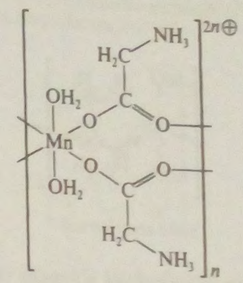
[59091-75-7]

Van Nickerk, J.N. *et al*, *Acta Crystallogr.*, 1953, **6**, 609 (*cryst struct*)
Narayana, P.A. *et al*, *Can. J. Phys.*, 1968, **46**, 325 (*uv-vis*)
Karnezos, M. *et al*, *J. Appl. Phys.*, 1979, **50**, 1856 (*magnetism*)

IC-004300

$C_4H_{14}MnN_2O_6^{2\oplus}$

Diaquabis(glycine)manganese(2+)



M 241.1 (ion)

Polymorphic. Monoclinic and orthorhombic forms grown from same aq. soln. The 2 forms differ in the arrangement of their polymeric chains. Synth. from aq. $MnBr_2$ and glycine (1:2) ratio.

Dibromide, dihydrate: Cryst. A trihydrate with the same space group as the dihydrate has been reported.

Pepinski, R. *et al*, *Phys. Rev.*, 1958, **110**, 1309 (*synth, cryst struct*)
Glowiak, T., *Acta Crystallogr., Sect. B*, 1978, **34**, 1980 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 259 (*rev, bibl*)

IC-004301

$C_4H_{14}N_2NiO_2^{2\oplus}$

Bis(2-aminoethanol)nickel(*II*)(2+)

$[Ni(NH_2CH_2CH_2OH)_2]^{2\oplus}$

M 180.8 (ion)

Their blue colour casts doubt on the assertion that salts of this ion have square planar geometry.

Dibromide: [16481-89-3].
$C_4H_{14}Br_2N_2NiO_2$ M 340.6
Blue compd. with 2 or 3 $H_2NCH_2CH_2OH$ molecules as ligands or lattice molecules.

Sulfate: [63622-56-0].
$C_4H_{14}N_2NiO_6S$ M 276.9
Blue solid.

Udovenko, V.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1967, **12**, 510.
Masoud, M.S., *J. Inorg. Nucl. Chem.*, 1977, **39**, 413.

IC-004302

$C_4H_{14}N_4NiO_4$

Diamminebis(glycinato)nickel(*II*), 8CI

Bis(*glycinato*)*diamminenickel*(II)

[16893-70-2]

$Ni(NH_3)_2(NH_2CH_2CO_2)_2$

M 240.8

Blue-violet solid. Compd. little reported.

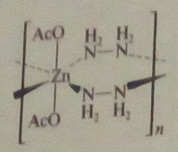
Becker, M.A. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 1288 (*synth, props, magnetism*)

$C_4H_{14}N_4O_4Zn$ IC-004303

Bis(acetato-*O*)bis(hydrazine)zinc

Dihydrazinezinc diacetate

[59922-97-3]



solid state struct.

M 247.5

In solid state, struct. comprises polymeric chains of 6-coord. Zn with H-bonding between CO and H_2N on adjacent chains. Cryst. (H_2O).

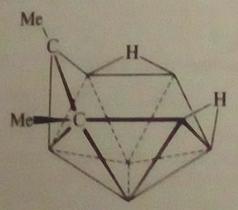
Ferrari, A. *et al*, *Acta Crystallogr.*, 1965, **19**, 548 (*synth, cryst struct*)

Patil, K.C., *Thermochim. Acta*, 1986, **99**, 153 (*synth, ir, thermal anal*)

Gudimovich, T.F. *et al*, *Zh. Obshch. Khim.*, 1988, 1449 (*phase diagram*)

$C_4H_{15}B_7$ IC-004304

4,5-Dimethyl-4,5-dicarbanonaborane(11)



M 138.8

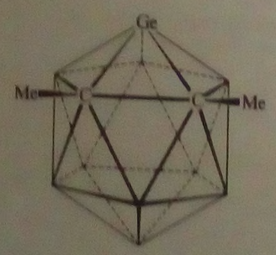
nido- Proposed structure. Synth. from B_5H_{12} with 2-butyne in Et_2O. Isol. by low temp. fractionation. Air-sensitive clear liq. Mp −9°

Schaeffer, R. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 1263 (*synth, ir, B-11 nmr, ms*)

$C_4H_{15}B_9Ge$ IC-004305

2,3-Dimethyl-1-germa-2,3-dicarbadodecaborane

[111876-64-3]



M 233.0

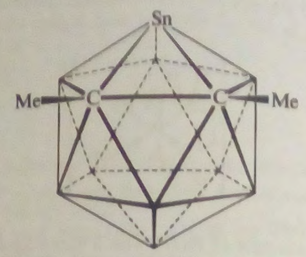
closo-. Colourless cryst. (by subl.). Mp 190° dec. $Subl._{0.0075}$ 100°.

Jutzi, P. *et al*, *J. Organomet. Chem.*, 1987, **319**, 139 (*synth, pmr, cmr, B-11 nmr, Sn-119 nmr, ms*)

$C_4H_{15}B_9Sn$ IC-004306

2,3-Dimethyl-1-stanna-2,3-dicarbadodecaborane

[95630-50-5]



M 279.1

closo-. Addition of ligands to the Sn moiety causes it to slip, becoming η^3-bound to B_1, B_2, B_3 (*nido*-). Air-sensitive colourless waxy cryst. (C_6H_6). Dec. at 190°.

THF complex: [107272-40-2].
$C_8H_{23}B_9OSn$ M 351.2
Cryst. Dec. at 138°. Adds another THF ligand reversibly in soln.

Bis-Py complex:
$C_{14}H_{25}B_9N_2Sn$ M 437.3
Air-sensitive colourless cryst. (CH_2Cl_2). Dec. at 190°.

Ph_3P complex:
$C_{22}H_{30}B_9PSn$ M 541.4
Dec. at 192°.

TMED complex:
$C_{10}H_{31}B_9N_2Sn$ M 395.3
Dec. at 247°.

Bipy complex: [95392-47-5].
$C_{14}H_{23}B_9N_2Sn$ M 435.3
Air-sensitive yellow cryst. + THF (THF). Sol. C_6H_6, THF. Dec. at 234°.

Phen complex:
$C_{16}H_{23}B_9N_2Sn$ M 459.3
Air-sensitive yellow solid. Dec. at 295°.

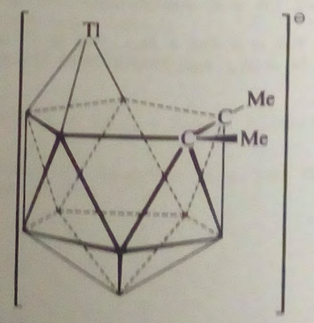
Jutzi, P. *et al*, *J. Organomet. Chem.*, 1987, **319**, 139 (*synth, pmr, cmr, B-11 nmr, Sn-119 nmr, ms*)

Jutzi, P. *et al*, *Organometallics*, 1987, **6**, 1024 (*derivs, cryst struct, pmr, B-11 nmr*)

$C_4H_{15}B_9Tl^{\ominus}$ IC-004307

[(7,8,9,10,11-η)-Nonahydro-7,8-dimethyl-7,8-dicarbaundecaborato(2−)]thallate(1−), 9CI

Nonahydro-2,3-dimethyl-1-thalla-2,3-dicarbadodecaborate(1−)



M 364.8 (ion)

Tl(1) *salt:* [41721-60-2].
$C_4H_{15}B_9Tl_2$ M 569.2

Colourless cryst. Sol. THF. Mp > 200°. Reacts with ROH giving $Tl[Me_2C_2B_9H_{10}]$.

Jutzi, P. *et al*, *Chem. Ber.*, 1991, **124**, 295 (*synth, pmr, B-11 nmr, cryst struct*)

$C_4H_{15}B_{10}ClHg$ IC-004308

[2-(Chloromethyl)-1,2-dicarbadodecaboran(12)-1-yl]methylmercury, 10CI, 9CI, 8CI

Chloromethyl(methylmercuri)-o-carborane.
Methyl(chloromethyl-o-carboranyl)mercury

[27378-38-7]

As Chloro(2-methyl-1,2-dicarbadodecaboran(12)-1-yl) mercury, IC-003727 with

$$R^1 = -HgMe,\ R^2 = -CH_2Cl$$

M 407.3

Cryst. Mp 122-122.5°.

Fedorov, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1970, 798 (*pmr, synth*)

Fedorov, L.A. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1970, **7**, 436 (*pmr*)

Stanko, V.I. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1973, **14**, 342 (*Cl-35 nqr*)

Fedorov, L.A., *J. Struct. Chem. USSR* (*Engl. Transl.*), 1976, **17**, 216 (*pmr*)

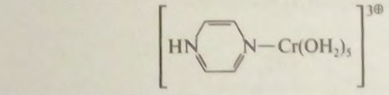
Bokii, N.G. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1978, **19**, 330 (*cryst struct*)

$C_4H_{15}CrN_2O_5^{3\oplus}$ IC-004309

Pentaaqua(pyrazinium)chromium(*III*)(3+)

Pentaaqua(pyrazine-N^1)chromium(2+), conjugate monoacid, 10CI. Pyrazine green

[73090-60-5]



M 223.1 (ion)

Cr(*III*)-pyrazine radical cation, stabilised by protonation of available nitrogen sites. Obt.from $[Cr(OH_2)_6]^{2\oplus}$ and pyrazine. Green. Esr-silent.

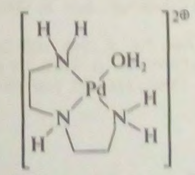
Dunne, T.G. *et al*, *Inorg. Chem.*, 1980, **19**, 1152 (*synth, uv-vis, esr*)

Swartz, J. *et al*, *Inorg. Chem.*, 1981, **20**, 2250 (*electrochem*)

$C_4H_{15}N_3OPd^{2\oplus}$ IC-004310

Aqua(diethylenetriamine)palladium(*II*)(2+)

[N-(2-*Aminoethyl*)-1,2-*ethanediamine*-N,N′,N″] *aquapalladium*(II)(2+), *9CI*



M 227.6 (ion)

Catalyses oxidative hydrolysis of olefins. Reacts with $BPh_4^{\ominus}$ to afford $[Pd(dien)Ph]^{\oplus}$.

Diperchlorate: [53773-88-9].
Yellow cryst. Sol. H_2O, Me_2CO, THF, Me_2CO. pK_a 7.1.
▷ Potentially explosive.

Burgess, C. *et al*, *J. Organomet. Chem.*, 1974, **76**, 247 (*synth, uv-vis, reaction*)

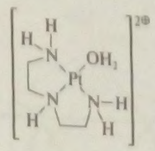
Chin, P.-K.F. *et al*, *Inorg. Chem.*, 1976, **15**, 982 (*synth, pmr, cmr*)

$C_4H_{15}N_3OPt^{2\oplus}$ IC-004311

Aqua(diethylenetriamine)platinum(*II*)(2+)

[N-(2-*Aminoethyl*)-1,2-*ethanediamine*]*aquaplatinum*(2+). *Aqua(1,4,7-triazaheptane)platinum*(II)

[48102-16-5]



M 316.2 (ion)

There is controversy over mechanism of replacement of H_2O.

Perchlorate: [42596-93-0].
Yellow-brown cryst. Sol. H_2O.
▷ Potentially explosive.

Gray, H.B. *et al*, *Inorg. Chem.*, 1962, **1**, 481 (*reactions*)

Alcock, R.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1070 (*synth*)

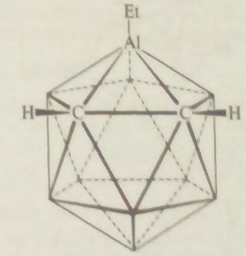
Beattie, J.K., *Inorg. Chim. Acta*, 1983, **76**, L69 (*reactions*)

$C_4H_{16}AlB_9$ IC-004312

3-Ethyl-3-aluminio-1,2-dicarba-*closo*-dodecaborane(12)

Ethyl[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]aluminium, 9CI

[34540-15-3]



M 188.4

Colourless cryst. (C_6H_6/hexane). Mp 97-99°.
▷ Explodes on contact with water.

Bis-THF adduct: [34540-18-6].
$C_{12}H_{33}AlB_9O_2$ M 332.6
Mp 119-120°.

Young, D.A.T. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, ir, pmr, nmr*)

Churchill, M.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1317 (*struct*)

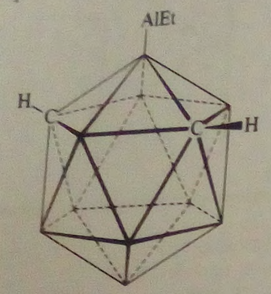
IC-004313

$_{16}AlB_9$

Ethyl-3-aluminio-1,7-dicarba-*closo*-dodecaborane(12)

thyl[(7,8,9,10,11-η)-undecahydro-7,9-arbaundecaborato(2−)]aluminium, 9CI

606-90-1]



188.4

> 100-102°.

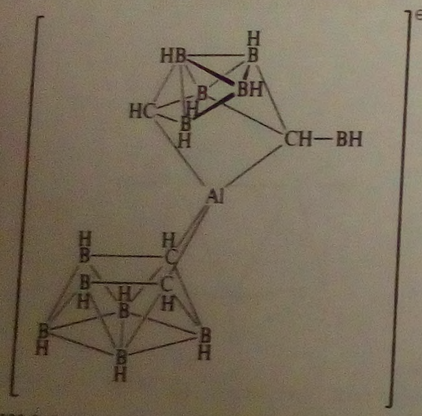
plodes with water.

ung, D.A.T. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, ir, nmr, nmr*)

IC-004314

$_{16}AlB_{12}^{\ominus}$

[3,5-dicarbaoctaborane(10)-3,5-diyl]aluminate(1−)



220.8 (ion)

antiomeric forms rapidly interconvert in toluene soln.

form

±)-form

salt: [108119-93-3].

$_4H_{16}AlB_{12}Na$ M 243.8

White air- and moisture-sensitive

ryst.(toluene/pentane). Ir ν_{BH} 2525 cm^{-1}. Forms Et_2O olvate.

119-94-4]

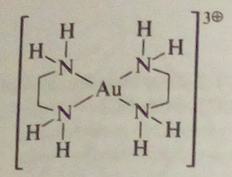
ubert, D.M. *et al*, *Organometallics*, 1987, **6**, 1353 (*synth, pmr, 1-11 nmr, ir, cryst struct*)

IC-004315

$C_4H_{16}AuN_4^{3\oplus}$

Bis(ethylenediamine)gold(*III*)(3+)

Bis(1,2-ethanediamine-N,N′)gold(3+), 11CI, 10CI



M 317.1 (ion)

Tribromide:

$C_4H_{16}AuBr_3N_4$ M 556.8

Pale yellow cryst. (H_2O).

Triperchlorate: [91321-06-1].

Synth. from $[AuCl_2en_2]Cl$, $HClO_4$ and $AgClO_4$.

Monoclinic snow-white cryst. $+1H_2O$. Sol. H_2O.

Tris-picrate: [91321-07-2].

Egg-yellow cryst.

[53934-40-0, 71393-64-1, 106219-85-6]

Block, B.P. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 4722 (*synth*)
Kim, J.-H. *et al*, *Inorg. Chem.*, 1979, **18**, 3145 (*reactions*)
Brown, D.H. *et al*, *Inorg. Chim. Acta*, 1979, **32**, 117 (*uv*)
Gladkaya, A.Sh. *et al*, *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1984, **10**, 445 (*derivs, synth, pe, esr, ir, pmr*)
Minacheva, L.Kh. *et al*, *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1986, **12**, 816 (*synth, cryst struct, perchlorate*)
Gladkaya, A.Sh. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1987, **36**, 2466 (*reactions, synth, deriv*)

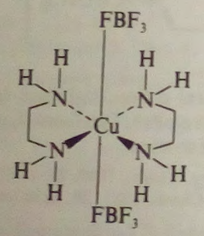
IC-004316

$C_4H_{16}B_2CuF_8N_4$

Bis(1,2-ethanediamine-*N,N′*)bis[tetrafluoroborato(1−)-*F*]copper(*II*), 11CI

Bis(ethylenediamine)copper(II) *fluoroborate*

[23730-93-0]



M 357.3

Elongated octahedral Cu with Cu—N 202-203, Cu—F 256 pm. Violet platelets.

[92419-37-9]

Brown, D.S. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 730 (*cryst struct*)
Procter, I.M. *et al*, *J. Chem. Soc. A*, 1968, 1678 (*synth*)
Hathaway, B.J. *et al*, *J. Chem. Soc. A*, 1969, 319 (*esr, uv-vis*)
Deeth, R.J. *et al*, *Inorg. Chem.*, 1984, **23**, 3846 (*uv-vis, theory*)

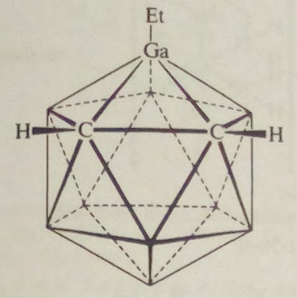
IC-004317

$C_4H_{16}B_9Ga$

3-Ethyl-3-galla-1,2-dicarbadodecaborane(12)

Ethyl[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]gallium, 9CI

[34540-17-5]



M 231.1

Struct. by analogy with Al analogue. Extremely air-sensitive solid. Mp 114-115° (sealed tube). Partly isom. on heating at 400° to 3-Ethyl-3-galla-1,7-dicarbadodecaborane(12), IC-004318.

Young, D.A.T. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, nmr, ir, pmr*)

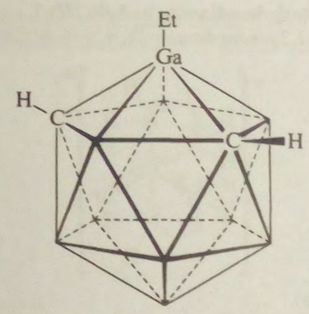
IC-004318

$C_4H_{16}B_9Ga$

3-Ethyl-3-galla-1,7-dicarbadodecaborane(12)

Ethyl[(7,8,9,10,11-η)-undecahydro-7,9-dicarbaundecaborato(2−)]gallium, 9CI

[34540-19-7]



M 231.1

Struct. assumed by analogy with Al analogue. Formed on heating 3-Ethyl-3-galla-1,2-dicarbadodecaborane(12), IC-004317 to 400°. Solid.

Young, D.A.T. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, nmr, ir, pmr*)

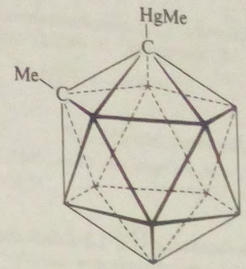
IC-004319

$C_4H_{16}B_{10}Hg$

Methyl(2-methyl-1,2-dicarbadodecaboran(12)-1-yl)mercury, 8CI

Methyl(methyl-o-carboranyl)mercury. 1-Methyl-2-methylmercuri-o-carborane. Methyl(methylbarenyl)mercury

[20643-84-9]



M 372.8

Cryst. (heptane). Mp 167-167.5°.

Zakharkin, L.I. *et al*, *J. Organomet. Chem.*, 1966, **6**, 228 (*synth*)
Fedorov, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1970, 798 (*pmr*)
Fedorov, L.A. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1971, **7**, 436 (*pmr*)

IC-004320

$C_4H_{16}B_{10}Hg$

Methyl(7-methyl-1,7-dicarbadodecaboran(12)-1-yl)mercury, 8CI

Methyl(methyl-m-carboranyl)mercury. 1-Methyl-7-methylmercuri-m-carborane. Methyl(methylneobarenyl)mercury

[23704-36-1]

As Dibromo-μ-1,7-dicarbadodecaboran(12)-1,7-diyldimercury, IC-003321 with

R^1 = —HgMe, R^2 = CH_3

M 372.8

Cryst. (hexane). Mp 123-124°.

Zakharkin, L.I. *et al*, *J. Organomet. Chem.*, 1967, **7**, 385 (*synth*)
Fedorov, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1970, 798 (*pmr*)
Fedorov, L.A. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1971, **7**, 436 (*pmr*)

IC-004321

$C_4H_{16}B_{10}Hg_2$

μ-1,2-Dicarbadodecaboran(12)-1,2-diyldimethyldimercury, 8CI

1,2-Dicarbadodecaboran(12)-1,2-diylbis(methylmercury). 1,2-Bis(methylmercuri)-o-carborane. 1,2-Bis(methylmercuri)barene

[27378-35-4]

As Chloro(2-methyl-1,2-dicarbadodecaboran(12)-1-yl)mercury, IC-003727 with

R^1 = R^2 = —HgMe

M 573.4

Solid. Mp 254-256°.

Fedorov, L.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1970, 798 (*synth, pmr*)
Fedorov, L.A. *et al*, *J. Org. Chem. USSR* (*Engl. Transl.*), 1971, **7**, 436 (*pmr*)
Fedorov, L.A. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1970, **17**, 216 (*pmr*)

$C_4H_{16}B_{10}Hg_2$ IC-004322

μ-1,7-Dicarbadodecaboran(12)-1,7-diyldimethyldimercury, 8CI

1,7-Dicarbadodecaboran(12)-1,7-diylbis(methylmercury). 1,7-Bis(methylmercuri)-m-carborane. 1,7-Bis(methylmercuri) neobarene

[23704-37-2]

As Dibromo-μ-1,7-dicarbadodecaboran(12)-1,7-diyldimercury, IC-003321 with

$R^1 = R^2 = -HgMe$

M 573.4

Cryst. (C_6H_6/heptane). Mp 235-237°.

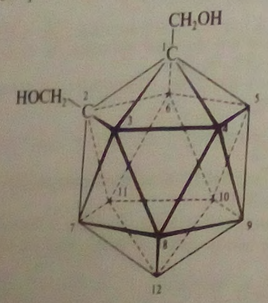
Zakharkin, L.I. *et al, J. Organomet. Chem.*, 1967, **7**, 385 (*synth*)

$C_4H_{16}B_{10}O_2$ IC-004323

1,2-Dicarbadodecaborane(12)-1,2-dimethanol, 10CI

1,2-Dimethylol-1,2-dicarbadodecaborane(12)

[19610-37-8]



M 204.2

closo-. Used in polyester carborane and polyurethane carborane syntheses. White solid (toluene). Mp 304°.

Heying, T.L. *et al, Inorg. Chem.*, 1963, **2**, 1097 (*synth*)
Fein, M.M. *et al, Inorg. Chem.*, 1963, **2**, 1115 (*synth*)
Green, J. *et al, J. Polym. Sci., Part A*, 1964, **2**, 3113 (*synth*)
Korshak, V.V. *et al, Vysokomol. Soedin., Ser. A*, 1970, **13**, 2137 (*synth*)
Bartet, B. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1974, **279**, 283, 593 (*ir, nmr*)

$C_4H_{16}B_{10}O_2$ IC-004324

1,7-Dicarbadodecaborane(12)-1,7-dimethanol, 10CI

1,7-Dimethylol-1,7-dicarbadodecaborane

[23924-78-9]

M 204.2

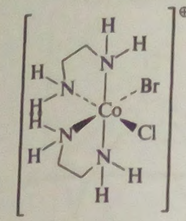
closo-. Used in polyester carborane and polyurethane carborane syntheses. White solid (toluene). Mp 194-196°.

Grafstein, D. *et al, Inorg. Chem.*, 1963, **2**, 1129 (*synth*)
Bartet, B. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1974, **279**, 283 (*ir*)

$C_4H_{16}BrClCoN_4^{\oplus}$ IC-004325

Bromochlorobis(ethylenediamine)cobalt(*III*)(1+)

Bromochlorobis(1,2-ethylenediamine-N,N′)cobalt(1+), 9CI



cis-form

M 294.4 (ion)

Prepd. by ligand substitution reactions.

cis-form [17611-36-8]

Bromide:

$C_4H_{16}Br_2ClCoN_4$ M 374.3

Dark grey powder. Insol. H_2O.

trans-form [17611-37-9]

Bromide: [16853-40-0].

Bright green cryst. V. sol. H_2O.

Nitrate: [15656-44-7].

Bright green cryst. Insol. H_2O.

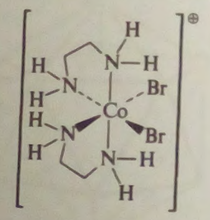
[16773-96-9, 28190-82-1, 32663-07-3]

Werner, A., *Justus Liebigs Ann. Chem.*, 1912, **386**, 1 (*synth*)
Chan, S.C. *et al, J. Chem. Soc.*, 1962, 4531 (*synth, hydrol*)
Inorg. Synth., 1967, **9**, 163 (*synth*)
Chottard, G., *Bull. Soc. Chim. Fr.*, 1973, 466 (*ir*)

$C_4H_{16}Br_2CoN_4^{\oplus}$ IC-004326

Dibromobis(ethylenediamine)cobalt(*III*)(1+)

Dibromobis(1,2-ethanediamine-N,N′)cobalt(III)(1+), 11CI



M 338.9 (ion)

cis-form

Bromide: [14911-27-4].

Charcoal grey cryst. + $1H_2O$ (olive green to maroon in soln.). Sol. H_2O. Hydrol. rapidly in acid soln. to mixture of *cis-* and *trans-*$[Co(en)_2(OH_2)Br]^{2\oplus}$.

trans-form [15379-04-1]

Bromide: [15005-14-8].

Light green cryst. More sol. than *cis*-form. First obtd. as unstable hydrobromide salt, ($2H_2O.HBr$).

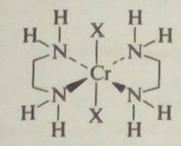
Werner, A., *Justus Liebigs Ann. Chem.*, 1912, **386**, 1 (*synth, isomers*)
Barraclough, C.G. *et al, Inorg. Chem.*, 1971, **10**, 1994 (*hydrol*)
Konovalov, L.V. *et al, Zh. Neorg. Khim.*, 1974, **19**, 89 (*ir*)
Warren, L.F. *et al, Inorg. Chem.*, 1976, **15**, 3126 (*uv-vis*)
Jackson, W.G. *et al, Inorg. Chem.*, 1978, **17**, 1348 (*synth, resoln, uv-vis*)
Chan, S.-Y. *et al, Croat. Chim. Acta*, 1979, **52**, 11 (*uv-vis*)
Kanamori, K. *et al, Bull. Chem. Soc. Jpn.*, 1980, **53**, 2520 (*raman*)
Inorg. Synth., 1982, **21**, 120 (*synth, isomers*)
Tsuchiya, R. *et al, Bull. Chem. Soc. Jpn.*, 1983, **56**, 2250 (*thermal stability*)

$C_4H_{16}Br_2CrN_4$ IC-004327

Dibromobis(ethylenediamine)chromium(*II*)

Dibromobis(1,2-ethanediamine-N,N′)chromium, 9CI

[17993-14-5]



X = Br

M 332.0

Presumed *trans*-octahedral. Violet air-sensitive cryst. Insol. org. solvs. except DMF. $\mu_{eff} = 4.74\mu_B$ (300K). Corresp. iodo compd. also known.

Larkworthy, L.F. *et al, J. Chem. Soc. A*, 1969, 1339 (*synth, props*)

$C_4H_{16}Br_2CrN_8S_4$ IC-004328

Dibromotetrakis(thiourea-*S*)chromium(*II*), 10CI

[74624-96-7]

$CrBr_2[S{=}C(NH_2)_2]_4$

M 516.2

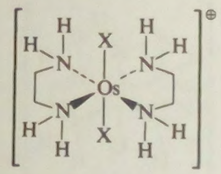
Distorted octahedral complex. Light blue solid. $\mu_{eff} = 4.86\mu_B$ (temp. independent).

Larkworthy, L.F. *et al, Inorg. Chim. Acta*, 1980, **40**, 217 (*synth, uv, ir*)

$C_4H_{16}Br_2N_4Os^{\oplus}$ IC-004329

Dibromobis(ethylenediamine)osmium(*III*)(1+)

Dibromobis(1,2-ethanediamine-N,N′)osmium(III)(1+), 9CI



X = Br

M 470.2 (ion)

trans-Octahedral.

Bromide: [57304-47-9].

Synth. from $[Os(en)_2H_2]^{2\oplus}$ + HBr in air.

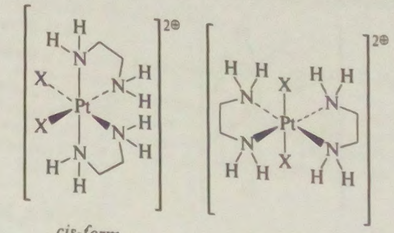
Coelho, A.L. *et al, Inorg. Chim. Acta*, 1975, **14**, L41 (*synth, uv, ir*)

$C_4H_{16}Br_2N_4Pt^{2\oplus}$ IC-004330

Dibromobis(ethylenediamine)platinum(*IV*), 8CI

Dibromobis(1,2-ethanediamine-N,N′)platinum(2+), 9CI

[62535-07-3]



cis-form *trans-form*

X = Br

M 475.0 (ion)

trans-form best known.

trans-form

Forms many salts with square planar $[ML_4]^{2\oplus}$ ions, having stacked structs. and one-dimensional electrical conductance.

Bis(ethylenediamine)platinum(2+) double salt, tetraperchlorate:

$C_8H_{32}Br_2Cl_4N_8O_{16}Pt_2$ M 1188.1

Green dichroic needles.

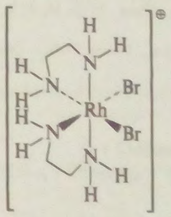
[82189-45-5, 87824-80-4]

Bekaroglu, O. *et al, Inorg. Chim. Acta*, 1977, **21**, 183 (*synth*)
Matsumoto, N. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 2334 (*uv-vis*)
Yamashita, M. *et al, Inorg. Chim. Acta*, 1978, **31**, L381 (*pe*)
Endres, H. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 35 (*cryst struct*)
Clark, R.J.H. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 579 (*raman*)

$C_4H_{16}Br_2N_4Rh^{\oplus}$ IC-004331

Dibromobis(ethylenediamine)rhodium(*III*)(1+)

Dibromobis(1,2-ethanediamine-N,N′)rhodium(III)(1+), 10CI



cis-form

M 382.9 (ion)

Pseudo-octahedral cation.

cis-form

Bromide: Yellow-orange solid.

Nitrate: [71701-38-7].

trans-form

Nitrate: [15529-89-2].

Orange solid. Sol. H_2O.

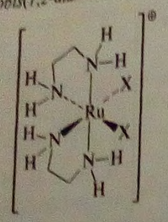
Johnson, S.A. *et al, Inorg. Chem.*, 1962, **1**, 925 (*synth, ir, uv*)
Ogino, M. *et al, Inorg. Chem.*, 1978, **17**, 1118 (*synth, uv*)

$C_4H_{16}Br_2N_4Ru^{\oplus}$ IC-004332

Dibromobis(ethylenediamine)ruthenium(*III*)(1+)

Dibromobis(1,2-ethanediamine-N,N′)ruthenium(1+), 9Cl

Dibromobis(1,2-diaminoethane)ruthenium(III)(*1+*)



cis-form

X = Br

M 381.0 (ion)

Sol. H_2O. The cation is readily hydrated for both isomers.

cis-form

Bromide: [15406-26-5].

Prepd. by treating corresp. $[RuBr_4(H_2NCH_2CH_2NH_2)]^{\ominus}$ salt with 1*M* HBr. Solid + $1H_2O$. $\mu_{eff} = 2.23\mu_B$; Ir $\nu_{Ru\text{-}Br}$ 207 cm^{-1}.

Perchlorate: [15406-27-6].

Prepd. by treating corresp. bromide with $NaClO_4$. Red cryst. Ir $\nu_{Ru\text{-}Br}$ 212 cm^{-1}.

▷ Potentially explosive.

Tetrabromo(ethylenediamine)ruthenate(1−) salt: [15406-28-7].

$C_6H_{24}Br_6N_6Ru_2$ M 861.8

Prepd. by treating $[Ru(en)_2(oxalato)^{\oplus}][Ru(en)(oxalato)_2^{\ominus}]$ with aq. HBr. Solid + $1H_2O$. $\mu_{eff} = 2.24\mu_B$ (per Ru atom). See also Tetrabromo(ethylenediamine) ruthenate(*III*)(1−), IC-003261.

trans-form [73238-27-4]

Bromide: [55870-35-4].

Yellow-brown cryst. Ir $\nu_{Ru\text{-}Br}$ 213 cm^{-1}.

[22294-94-6, 55822-57-6]

Broomhead, J.A. *et al, J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, magnetism, hydration*)

Broomhead, J.A. *et al, Inorg. Chem.*, 1975, **14**, 2575 (*synth, ir, uv, hydration*)

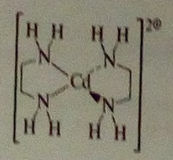
Poon, C.-K. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 128, 754 (*electrochem, synth*)

$C_4H_{16}CdN_4^{2\oplus}$ IC-004333

Bis(ethylenediamine)cadmium(2+)

Bis(1,2-ethanediamine-N,N′)cadmium(2+), 9Cl

[15552-66-6]



M 232.6 (ion)

Formed in solns. of $Cd^{2\oplus}$ containing ethylenediamine.

Schaap, W.B. *et al, J. Am. Chem. Soc.*, 1961, **83**, 4699 (*formn const*)

Fujita, T. *et al, Bull. Chem. Soc. Jpn.*, 1980, **53**, 930 (*struct, soln*)

$C_4H_{16}CdN_8S_4^{2\oplus}$ IC-004334

Tetrakis(thiourea-*S*)cadium(2+)

[23683-04-7]

$[(H_2N)_2C{=}S]_4Cd^{2\oplus}$

M 416.8 (ion)

Coordination is through the S atom. No phys. props. reported.

[19596-78-2, 19596-80-6]

Lane, T.J. *et al, J. Am. Chem. Soc.*, 1958, **80**, 315 (*formn, const*)

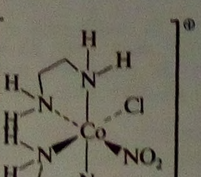
Flint, C.D. *et al, J. Chem. Soc. A*, 1967, 1718 (*synth, ir*)

$C_4H_{16}ClCoN_4O_3S$ IC-004335

Chlorobis(ethylenediamine)sulfitocobalt(*III*)

Chlorobis(1,2-ethanediamine-N,N′)[sulfito(2−)-S]cobalt, 10Cl

[73948-85-3]



M 294.6

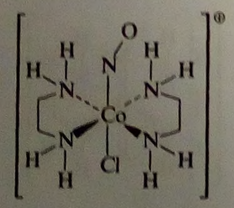
trans-Octahedral with long Co—Cl at ~238 pm. Red-brown cryst. + $1H_2O$. Sol. H_2O.

Baldwin, M.E., *J. Chem. Soc.*, 1961, 3123 (*synth, ir*)

Raston, C.L. *et al, Aust. J. Chem.*, 1980, **33**, 419 (*cryst struct*)

$C_4H_{16}ClCoN_5O^{\oplus}$ IC-004336

Chlorobis(ethylenediamine)nitrosylcobalt(1+), 8Cl



M 244.5 (ion)

Approx. *trans*-octahedral at Co with bent NO.

Perchlorate: [28067-89-2].

Brown solid. Sol. $MeNO_2$.

▷ Potentially explosive.

Feltham, R.D. *et al, Inorg. Chem.*, 1965, **4**, 1334 (*synth, ir, props*)

Synder, D.A. *et al, Inorg. Chem.*, 1970, **9**, 2760 (*cryst struct*)

$C_4H_{16}ClCoN_5O_2^{\oplus}$ IC-004337

Chlorobis(ethylenediamine)nitritocobalt(*III*)(1+)

Chlorobis(1,2-ethanediamine-N,N′)(nitrito-N)cobalt(1+), 9Cl. Chlorobis(ethylenediamine)nitrocobalt(1+), 8Cl

M 260.5 (ion)

cis-form [16884-74-5]

Chloride: [14221-34-2].

Orange-red cryst.

trans-form [16884-75-6]

Chloride: [14221-04-6].

Pale-red leaflets.

[14221-03-5, 15670-56-1]

Werner, A., *Ber.*, 1901, **34**, 1733, 1739 (*synth*)

Hughes, M.N. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 1659 (*ir*)

Lantzke, I.R. *et al, Aust. J. Chem.*, 1967, **20**, 35 (*pmr*)

Kanamori, K. *et al, Bull. Chem. Soc. Jpn.*, 1980, **53**, 2520 (*raman*)

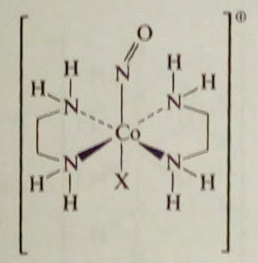
Rindermann, W. *et al, Inorg. Chim. Acta*, 1982, **64**, L203 (*synth, aquation*)

Odaka, Y. *et al, Bull. Chem. Soc. Jpn.*, 1985, **58**, 3407 (*N-15 nmr*)

$C_4H_{16}ClCoN_5O_5^{\oplus}$ IC-004338

Bis(ethylenediamine)nitrosylperchloratocobalt(1+)

Bis(1,2-ethanediamine-N,N′)nitrosyl(perchlorato-O) cobalt(1+), 9Cl



X = $OClO_3$

M 308.5 (ion)

trans-Octahedral config. with strongly bent NO group and monodentate $ClO_4^{\ominus}$.

Perchlorate: [60384-76-1].

Black cryst. Sol. $MeNO_2$.

[39721-22-7]

Feltham, R.D. *et al, Inorg. Chem.*, 1965, **4**, 1334 (*synth, ir*)

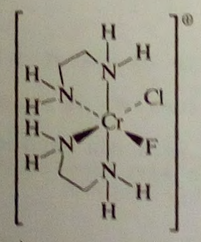
Johnson, P.L. *et al, Inorg. Chem.*, 1976, **15**, 2989 (*cryst struct*)

$C_4H_{16}ClCrFN_4^{\oplus}$ IC-004339

Chlorobis(ethylenediamine)fluorochromium(*III*)(1+), 8Cl

Chlorobis(1,2-ethanediamine-N,N′)fluorochromium(1+), 11Cl, 10Cl

[42476-29-9]



cis-form

M 226.6 (ion)

(+),*cis-form*

Bromide: [19605-18-6].

Purple cryst. + 0.25 EtOH. $[\alpha]_D$ +191° (0.1%).

(±),*cis-form*

Chloride: [19581-09-0].

Hygroscopic purple cryst. + $1H_2O$. Ir $\nu_{Cr\text{-}N}$ 490, 445, 420, ν_{CrF} 355, ν_{CrCl} 320 cm^{-1}.

Iodide: [62792-37-4].

Purple cryst.

Perchlorate: [62792-41-0].

Purple solid.

trans-form

Perchlorate: [26748-18-5].

Cryst. (aq. $NaClO_4$).

[62792-40-9]

Vaughn, J.W. *et al, Inorg. Chem.*, 1968, **7**, 736; 1970, **9**, 684 (*synth, resoln, cis-form*)

Wirth, G. *et al, Inorg. Chem.*, 1973, **12**, 1955 (*synth, trans-form*)

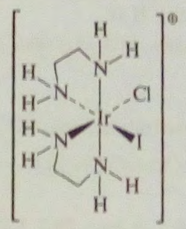
DeJovine, J.M. *et al, Inorg. Chem.*, 1974, **13**, 66 (*acid hydrol*)

Wong, C.F.C. *et al, Inorg. Chem.*, 1977, **16**, 3148 (*photol*)

Vaughn, J.W. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1977, **7**, 165.

$C_4H_{16}ClIrN_4^{\oplus}$ IC-004340

Chlorobis(ethylenediamine)iodoiridium(*III*)(1+)



cis-form

M 474.7 (ion)

Octahedral geometry.

cis-form

Nitrate: [35762-48-2].

Bright yellow solid.

trans-form

Obt. from *trans*-$[Ir(ethylenediamine)_2Cl_2](ClO_4)$ and NaI under uv light. Misprinted in the original paper as *trans*-$[Ir(ethylenediamine)Cl](ClO_4)$.

Perchlorate: [21210-18-4].

Sol. H_2O.

▷ Potentially explosive.

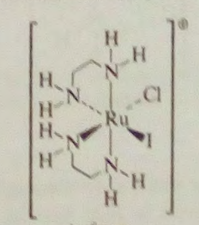
Bauer, R.A. *et al, Inorg. Chem.*, 1969, **8**, 2231 (*synth, uv*)

Nefedov, V.I. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1972, **17**, 244 (*synth, pe*)

$C_4H_{16}ClIN_4Ru^{\oplus}$ IC-004341

Chlorobis(ethylenediamine)iodoruthenium(*III*)(1+), 8Cl

Chlorobis(1,2-ethanediamine-N,N′)iodoruthenium(III)(*1+*)



cis-form

M 383.6 (ion)

Sol. H_2O.

Iodide: [15406-30-1].

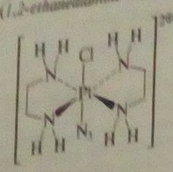
Prep. by treating Dichlorobis(ethylenediamine) ruthenium(1+), IC-004335? with aq. KI. Dark purple solid + $1H_2O$. Ir $\nu_{Ru\text{-}Cl}$ 303 cm^{-1}.

Broomhead, J.A. *et al, J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv*)

$C_4H_{10}ClN_2Pt^{2\oplus}$ IC-004342

Azidochlorobis(ethylenediamine)platinum(*IV*)

Azidochlorobis(1,2-ethanediamine-N,N')platinum(2+), 9CI



M 392.7 (ion)

trans-form

Synth. from *trans*-form of Dichlorobis(ethylenediamine) platinum(*IV*)(2+), IC-004355 + $N_3^{\ominus}$.

Dichloride: [54566-85-7].
$C_4H_{10}Cl_2N_8Pt$ M 463.6
Lemon yellow cryst. Sol. H_2O.

Bryan, H.A. *et al, Inorg. Chem.*, 1975, **14**, 1336.

$C_4H_{10}ClN_9S_4Tc^{\oplus}$ IC-004343

Chlorotetrakis(thiourea)nitridotechnetium(*V*)(1+)

$[N{\equiv}TcCl[S{=}C(NH_2)_2]_4]^{\oplus}$

M 452.8 (ion)
Synth. from $TcO_4^{\ominus}$ + $N_3^{\ominus}$ in conc. HCl. Useful synthetic intermed. for other complexes with Tc≡N core (e.g. Nitridobis(8-quinolinethiolato-N^1,S^8)technetium(*V*), IC-009766).

Chloride: [114368-22-8].
Orange cryst. (EtOH aq. containing excess thiourea). Sol. H_2O. Mp 210-212°.

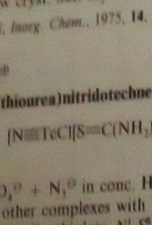
Baldas, J. *et al, Inorg. Chim. Acta*, 1988, **141**, 153 (*synth, ir, props*)

$C_4H_{10}Cl_2CoN_4^{\oplus}$ IC-004344

Dichlorobis(ethylenediamine)cobalt(*III*)(1+)

Dichlorobis(1,2-ethanediamine-N,N')cobalt(III)(1+), *9CI*

[15275-04-4]



cis-form

M 250.0 (ion)

cis-form

Can be resolved with e.g. bromocamphor sulfonate.

Chloride: Purple cryst. + H_2O. Less sol. than *trans*-form.

trans-form

Chloride: [14040-33-6].
Dark green cryst. Aquates in H_2O.

Chloride, HCl.2H$_2$O complex: [58298-19-4].
Green cryst.

Perchlorate: [14407-65-9].
Formed in thermal hydrolysis of $[Co(en)_2CO_3]^{\oplus}$ in HCl soln. Green cryst.

Tetrachlorothallate(1−): [41133-28-2].
Green cryst.

Tetrachlorocobaltate(2−) (2:1): [77289-74-8].
Green cryst. Sol. H_2O. μ_{eff} = 3.71 μ_B. Mixed valency compd., paramagnetic owing to $Co^{2\oplus}$.

[14403-91-9, 14875-15-1, 18660-62-3, 45837-15-8]

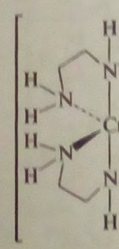
Inorg. Synth., 1946, **2**, 222; 1973, **14**, 68 (*synth, uv-vis, resoln*)
Ooi, S. *et al, Bull. Chem. Soc. Jpn.*, 1959, **32**, 263; 1963, **36**, 1083 (*synth, trans-form*)
Gillard, R.D. *et al, J. Chem. Soc.*, 1964, 1640 (*synth, trans-form*)
Matsumoto, K. *et al, Bull. Chem. Soc. Jpn.*, 1970, **43**, 3801 (*cis-form, cryst struct*)
Sharrock, P., *J. Chem. Educ.*, 1980, **57**, 778 (*synth*)
Schubert, V. *et al, Cryst. Struct. Commun.*, 1981, **10**, 239 (*cryst struct, trans-form*)
Rindermann, W. *et al, Inorg. Chim. Acta*, 1982, **64**, 2203 (*synth*)
Niederhoffer, E.C. *et al, Acta Crystallogr., Sect. C*, 1986, **42**, 568 (*cryst struct, trans-form*)

$C_4H_{10}Cl_2CrN_4^{\oplus}$ IC-004345

Dichlorobis(ethylenediamine)chromium(*III*)(1+), 8CI

Dichlorobis(1,2-ethanediamine-N,N')chromium(III) *(1+), 11CI, 10CI, 9CI*

[31303-32-9]



cis-form

M 243.0 (ion)
Pseudooctahedral cation. Many salts known.

cis-form [14482-74-7]

Chloride: [14240-29-0].
$C_4H_{10}Cl_3CrN_4$ M 278.5
Red-violet needles + $1H_2O$ (aq. HCl). Sol. H_2O, slowly dec,.

Bis(diethylphenylphosphine)tetrakis(thiocyanato-N) chromate(1−): [96491-66-6].
$C_{28}H_{46}Cl_2Cr_2N_8P_2S_4$ M 859.8

trans-form [14403-88-4]

Chloride: [14301-97-4].
Green cryst. + H_2O or bluish green dichroic tablets + HCl + $2H_2O$. Sol. H_2O.

Perchlorate: [15654-82-7].
Solid. Insol. H_2O.

[42281-19-6]

Ooi, S. *et al, Bull. Chem. Soc. Jpn.*, 1960, **33**, 354 (*cryst struct, chloride, trans-form*)
Pedersen, E., *Acta Chem. Scand.*, 1970, **24**, 3362 (*synth, cis chloride*)
Fee, W.W. *et al, J. Chem. Soc. A*, 1970, 2612 (*synth, trans salts*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1501 (*synth*)

$C_4H_{16}Cl_2CrN_8O_4$ IC-004346

Dichlorotetrakis(urea-*O*)chromium(*II*), 10CI

Chromium(II) *chloride tetrakis(urea)*

[67607-22-1]

$CrCl_2[O{=}C(NH_2)_2]_4$

M 363.1

Distorted 6-coord. monomer. Synth. from urea and $CrCl_2.4H_2O$ in EtOH/2,2-dimethoxypropane. Blue air-sensitive microcryst. μ_{eff} = 4.78μ_B (295K), 4.83μ_B (90K). Corresp. Br complex also known.

Larkworthy, L.F. *et al, Inorg. Chim. Acta*, 1978, **28**, 251 (*uv-vis, ir, magnetism, synth*)

$C_4H_{16}Cl_2CrO_4^{\oplus}$ IC-004347

Dichlorotetrakis(methanol)chromium(*III*)(1+), 9CI

[55954-66-0]

$[CrCl_2(MeOH)_4]^{\oplus}$

M 251.0 (ion)
trans-Octahedral with Cr—Cl 228.8, 230.2, Cr—O 198.7 pm.

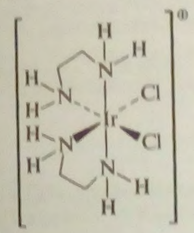
Chloride: Chromium(III) *chloride tetrakis-methanol*
$C_4H_{16}Cl_3CrO_4$ M 286.5
From $CrCl_3.6H_2O$ and 2,2-dimethoxypropane; then evaporation at 75°, or $CrCl_3(THF)_3$ and MeOH. Green cryst. (MeOH at 5°). Sol. MeOH. Dec. to $CrCl_3(MeOH)_3$ at *ca.* 120°.

Hardcastle, K.I. *et al, J. Chem. Soc., Chem. Commun.*, 1975, 190 (*cryst struct*)
Mehrotra, R.C. *et al, Transition Met. Chem.*, 1977, **2**, 161 (*synth, vis, ir, esr*)

$C_4H_{16}Cl_2IrN_4^{\oplus}$ IC-004348

Dichlorobis(ethylenediamine)iridium(*III*)(1+), 8CI

Dichlorobis(1,2-ethanediamine-N,N')iridium(1+)



cis-form

M 383.3 (ion)

cis-form

Chloride: [15444-47-0].
Yellow cryst. Sp. sol. cold H_2O.

Perchlorate: Yellow cryst.
▷ Potentially explosive.

trans-form

Chloride: [15444-46-9].
Yellow solid. Sol. H_2O.

Perchlorate: Yellow cryst. Sol. H_2O.
▷ Potentially explosive.

Kida, S. *et al, Bull. Chem. Soc. Jpn.*, 1966, **39**, 2415 (*synth, ir*)
Bauer, R.A. *et al, Inorg. Chem.*, 1969, **8**, 2231 (*synth, uv*)
Galsbol, F. *et al, Acta Chem. Scand., Ser. A*, 1982, **36**, 439 (*synth, uv*)

$C_4H_{16}Cl_2MnN_4$ IC-004349

Dichlorobis(ethylenediamine)manganese

Dichlorobis(1,2-ethanediamine-N,N')manganese(II).
Manganese(II) *chloride bis(ethylenediamine)*

[52572-34-6]

$MnCl_2(H_2NCH_2CH_2NH_2)_2$

M 246.0

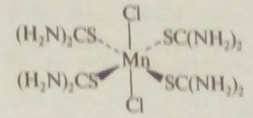
Synth. from anhydrous $MnCl_2$ in dry EtOH and $H_2NCH_2CH_2NH_2$ in C_6H_6. White powder, stable at 25° in a dry atm., dec. by boiling H_2O.

Prasad, S. *et al, J. Indian Chem. Soc.*, 1958, **35**, 722 (*synth, magnetism*)
Syamal, A., *J. Inst. Chem. (India)*, 1968, **40**, 102 (*magnetism*)
Chiswell, B. *et al, Inorg. Chim. Acta*, 1973, **7**, 707 (*synth*)

$C_4H_{16}Cl_2MnN_8S_4$ IC-004350

Dichlorotetrakis(thiourea-*S*)manganese(*II*), 11CI

[14240-54-1]



M 430.3
trans-Octahedral. Synth. from $MnCl_2$ and thiourea (1:4 ratio) in hot EtOH. White or v. pale green cryst. (EtOH). Sol. Me_2CO, $PhNO_2$. Mp 193-195°. μ_{eff} = 5.9μ_B. Solns. aquate in H_2O.

Flint, C.D. *et al, J. Chem. Soc. A*, 1966, 744 (*synth, ir*)
Ashcroft, S.J., *J. Chem. Soc. A*, 1970, 1020 (*thermodynamics*)
Gerloch, M. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1559 (*magnetism*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1967, 884 (*ir*)
Dremyatskaya, L.D. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1090 (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 187 (*rev, bibl*)

$C_4H_{16}Cl_2N_4Ni$ IC-004351

Dichlorobis(ethylenediamine)nickel(*II*)

Bis(ethylenediamine)nickel chloride. Dichlorobis(1,2-ethanediamine-N,N')nickel

[22980-82-1]

$(H_2NCH_2CH_2NH_2)_2NiCl_2$

M 249.7
Compd. of this apparent formula is really the chloride salt of Di-μ-chlorotetrakis(ethylenediamine)dinickel(*II*)(2+), IC-006350.

[88196-50-3]

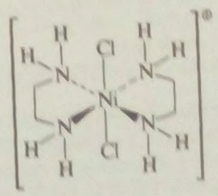
Antsyshkina, A.S. *et al, Dokl. Akad. Nauk SSSR*, 1962, **143**, 105; *CA*, 1962, **57**, 2954f (*struct*)

$C_4H_{16}Cl_2N_4Ni^{\oplus}$ IC-004352

Dichlorobis(ethylenediamine)nickel(*III*)(1+), 8CI

Dichlorobis(1,2-ethanediamine-N,N')nickel(III)(1+), *9CI*

[29806-10-8]



M 249.7 (ion)
trans-struct. Exists as both Ni(*III*) and Ni(*II,IV*) mixed valence forms, often as mixts., with much literature confusion.

Chloride: [23970-35-6].
$C_4H_{16}Cl_3N_4Ni$ M 285.2

Perchlorate: [14587-76-9].

$C_4H_{16}Cl_2N_4Os^{\oplus} - C_4H_{16}Cl_2N_4Rh^{\oplus}$

$C_4H_{16}Cl_2N_4NiO_4$ M 349.2
▷ Potentially explosive.

Nickel(III)-form
Has linear polymeric struct. Salts are brown-yellow.

Nickel(II,IV)-form
Tetrachlorotetrakis(ethylenediamine)dinickel(II,IV)
[Dichlorobis(1,2-ethanediamine)nickel][dichlorobis(1,2-ethanediamine)nickel(2+)]
Has linear polymeric struct. Possesses high electrical conductance similar to chloride salt of [Dichlorobis(1,2-propanediamine)nickel(2+)][bis(1,2-propanediamine)nickel(2+)]. IC-008334. Salts are green-black.

[20540-40-3, 55157-09-0, 80419-90-5, 84277-66-7]

Cooper, D.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2131.
Yamashita, M. *et al*, *Inorg. Chim. Acta*, 1985, **97**, L43.

$C_4H_{16}Cl_2N_4Os^{\oplus}$ IC-004353

Dichlorobis(ethylenediamine)osmium(*III*)(1+)
Dichlorobis(1,2-ethanediamine-N,N′)osmium(III)(*1+*)

[79573-09-4]

As Dibromobis(ethylenediamine)osmium(*III*)(1+), IC-004329 with

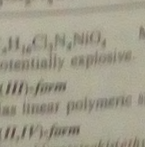
X = Cl

M 381.3 (ion)
trans-Octahedral.
Chloride: [57335-17-8].
Synth. from $[Os(en)_2H_2]^{2\oplus}$ + aq. HCl in air.
Perchlorate: [79573-10-7].
Synth. by reaction of $Na_2[OsCl_6]$, $Na[H_2PO_2]$ and ethylenediamine in MeOH followed by addition of $Na[ClO_4]$. Yellow solid. $\mu_{eff} = 2.05\mu_B$ (r.t.).

Coelho, A.L. *et al*, *Inorg. Chim. Acta*, 1975, **14**, L41 (*synth, ir, uv*)
Poon, C.-K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1697 (*synth, uv*)

$C_4H_{16}Cl_2N_4Pd^{2\oplus}$ IC-004354

Dichlorobis(ethylenediamine)palladium(*IV*)(2+)



trans-form

M 297.5 (ion)
Generally obt. with *trans*-geometry. Simple salts unstable, cation more stable in mixed valence compds.
Diperchlorate: [36245-59-7].
Light yellow-green cryst.
Dinitrate, double salt with $[Pd(en)_2](NO_3)_2$: Synth. from $[Pd(en)_2]Cl_2$ and HNO_3. Dark green cryst. Previously formulated as simple nitrate.
Diperchlorate, double salt with $[Pd(en)_2](ClO_4)_2$: [73857-02-0].
Synth. from $[Pd(en)_2]Cl_2$, $HClO_4$ and Cl_2. Green cryst. with metallic lustre (cold aq. $HClO_4$). Solid, but not soln., shows strong absorption in visible region due to charge transfer from Pd(*II*) to Pd(*IV*) along Pd(*II*)...Cl...Pd(*IV*).

[67825-21-2]

Babaeva, A.V. *et al*, *Zh. Neorg. Khim.*, 1967, **12**, 393 (*cis?-form*)
Mason, W.R., *Inorg. Chem.*, 1973, **12**, 20 (*synth, perchlorate, mixed valence derivs, uv*)
Matsumoto, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1978, **51**, 2334 (*synth, mixed valence derivs, uv*)
Papavassiliou, G.C. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1981, **77**, 191 (*uv, raman, mixed valence derivs*)

$C_4H_{16}Cl_2N_4Pt^{2\oplus}$ IC-004355

Dichlorobis(ethylenediamine)platinum(*IV*)(2+)
Dichlorobis(1,2-ethanediamine-N,N′)platinum(2+), 9Cl

As Dibromobis(ethylenediamine)platinum(*IV*), IC-004330 with

X = Cl

M 386.1 (ion)
cis-form [19184-32-8]
Chiral.
Dichloride: [17374-56-0].
$C_4H_{16}Cl_4N_4Pt$ M 457.0
White cryst.
trans-form [29646-65-9]
Forms many double salts with square planar $M^{2\oplus}$ ions, giving stacked structures and 1-dimensional electrical conductance.
Chloride: [16924-88-2].
Yellow solid.
Bis(ethylenediamine)platinum(2+) double salt, tetraperchlorate: [67825-38-1].
$C_8H_{32}Cl_6N_8O_{16}Pt_2$ M 1099.2
One-dimensional conductor. Purple or red cryst.
▷ Potentially explosive.

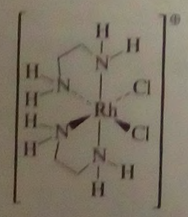
[17374-56-0, 21430-85-3, 28491-18-1]

Liu, C.F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 412 (*synth, ir, pmr, ord, cis*-form)
Liu, C.F. *et al*, *Inorg. Chem.*, 1970, **9**, 773 (*cryst struct, cis*-form)
Tanaka, M. *et al*, *Chem. Phys.*, 1985, **96**, 343 (*ir, uv, raman, trans*-form)

$C_4H_{16}Cl_2N_4Rh^{\oplus}$ IC-004356

Dichlorobis(ethylenediamine)rhodium(*III*)(1+)
Dichlorobis(1,2-ethanediamine-N,N′)rhodium(III)(*1+*)

[29701-59-5]



cis-Λ-form

M 294.0 (ion)
Well studied example of *cis/trans* isomerism.
cis-Λ-form [65830-10-6]
cis-(−)-*form*
Config. assigned by comparison of cd data with that of Λ-Co[$(en)_2Cl_2$]$^{\oplus}$. $[\alpha]_{435}$ −58°, $[\alpha]_{577}$ −50°.
cis-Δ-form [64598-97-6]
cis-(+)-*form*
$[\alpha]_{89}$ +216°.
cis-form [24444-43-7]
cis-(±)-*form*
Nitrate: [39561-32-5].
Bright yellow cryst. (conc. HNO_3). Sol. hot H_2O. Layer struct, en ligands have gauche config.
Chloride: [15444-62-9].

Yellow cryst. + $1H_2O$ (conc. HCl). V. sol. H_2O; sol. DMSO. Loses H_2O on heating at 100° for 30 mins.
Perchlorate: [67047-30-7].
Synth. from the chlorides and 60% $HClO_4$. Yellow cryst.
trans-form [18539-17-8]
Nitrate: [15529-88-1].
Golden yellow, or orange cryst. (conc. HNO_3). Sol. H_2O. Monoclinic, distorted NaCl struct.
Chloride: [15444-63-0].
Yellow cryst. + H_2O (conc. HCl). V. sol. H_2O; sol. DMSO. Loses H_2O on heating at 100° for ½ hour.
Perchlorate: [41367-59-3].
Cryst. Sol. H_2O. Ir ν_{RuCl} 344 vs cm^{-1} (nujol). Raman ν_{RuCl} 305 vs cm^{-1}.

[34768-40-6, 103937-70-8]

Johnson, S.A., *Inorg. Chem.*, 1962, **1**, 925 (*synth, uv, resoln, chloride, ir*)
Inorg. Synth., 1963, **7**, 214; 1980, **20**, 57; 1986, **24**, 283 (*synth*)
Gillard, R.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1241 (*abs config, cd*)
Ogino, H. *et al*, *Inorg. Chem.*, 1978, **17**, 1118 (*uv-vis, cd, abs config*)
Jakse, F.P. *et al*, *Inorg. Chim. Acta*, 1978, **27**, 225 (*emr*)
Baidina, I.A. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1979, **20**, 934 (*cryst struct, NO_3*)
Gmelin Handbook Inorg. Chem., Syst. No. 64, Suppl., 1984, **B2**, 177 (*rev*)
Lynde-Kernell, T. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 31 (*cryst struct, NO_3*)

$C_4H_{16}Cl_2N_4Ru^{\oplus}$ IC-004357

Dichlorobis(ethylenediamine)ruthenium(1+)
Dichlorobis(1,2-ethanediamine-N,N′)ruthenium(1+), 9Cl
Dichlorobis(1,2-diaminoethane)ruthenium(III)

As Dibromobis(ethylenediamine)ruthenium(*III*)(1+), IC-004332 with

X = Cl

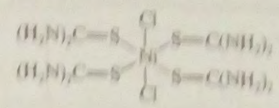
M 292.1 (ion)
Sol. H_2O. Both isomers are readily hydrated, thermally and photochemically.
cis-form [38687-00-2]
Chloride: [22294-93-5].
Prepd. by treating corresp. $[RuCl_4(H_2NCH_2CH_2NH_2)]^{\ominus}$ salt with 1*M* HCl. Orange cryst. + $1H_2O$. μ_{eff} = $2.13\mu_B$; Ir ν_{RuCl} 311, 273 cm^{-1}.
▷ VM2651200.
Tetrachloro(1,2-ethylenediamine)ruthenate(1−) salt: [15406-24-3].
$C_6H_{24}Cl_6N_6Ru_2$ M 595.1
Prepd. by treating $[Ru(en)_2(oxalato)^{\oplus}][Ru(en)(oxalato)_2^{\ominus}]$ with conc. HCl. Orange-red cryst. + $2H_2O$. $\mu_{eff} = 2.18\mu_B$ (per Ru atom).
trans-form [45839-20-1]
Chloride: [55822-58-7].
Prepd. by the thermal isom. of corresp. *cis* compd., followed by ion-exchange chromatogr. Orange cryst. + $\frac{1}{2}H_2O$. Ir ν_{RuCl} 325 cm^{-1}.
Iodide: [55822-59-8].
Prepd. by metathesis. Red cryst. + $\frac{1}{2}H_2O$.
Perchlorate: [56172-97-5].
Prepd. by heating $K_2[RuCl_5(OH_2)]$ in MeOH with $NH_2CH_2CH_2NH_2$ for several days, followed by $HClO_4$. Orange cryst. $\mu_{eff} = 2.23\mu_B$; Ir ν_{RuCl} 328 cm^{-1}.
▷ Potentially explosive.

[41509-67-5]

Broomhead, J.A. *et al*, *J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, magnetism, hydration*)
Broomhead, J.A. *et al*, *Inorg. Chem.*, 1973, **14**, 2575 (*synth, ir, uv, hydration*)
Chan, P.K. *et al*, *Inorg. Chem.*, 1975, **14**, 2579 (*synth, ir, magnetism, uv*)
Poon, C.-K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2115; 1978, 740; 1980, 128, 754; 1981, 2556 (*hydration, electrochem, synth*)
Rerek, M.E. *et al*, *Inorg. Chem.*, 1980, **19**, 2646 (*photolysis*)
Ceulemans, A. *et al*, *Inorg. Chem.*, 1983, **22**, 1113 (*photochem*)

$C_4H_{16}Cl_2N_8NiS_4$ IC-004358

Dichlorotetrakis(thiourea)nickel(*II*), 8Cl
Nickel(II) *chloride tetrakis(thiourea)*
[14840-53-0]



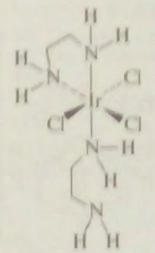
M 434.0
Octahedral. Paramagnetic.
trans-form
Yellow-brown cryst.

[28813-19-6, 80374-80-7]

Lopez-Castro, A. *et al*, *J. Chem. Soc.*, 1963, 1309 (*cryst struct*)
Adams, D.M. *et al*, *J. Chem. Soc. A*, 1967, 884 (*ir*)
Gerloch, M. *et al*, *J. Chem. Soc. A*, 1971, 2434 (*synth, uv, magnetism*)
Kharitonov, Y.Y. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 1187 (*ir*)
Srinivasan, V. *et al*, *Inorg. Chim. Acta*, 1977, **25**, L85 (*pe*)

$C_4H_{16}Cl_3IrN_4$ IC-004359

Bis(ethylenediamine)trichloroiridium(*III*)
Trichloro(1,2-ethanediamine-N)(1,2-ethanediamine-N,N′) iridium, 11Cl



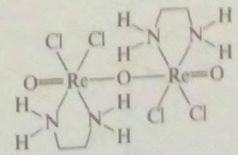
M 418.7
mer-Octahedral. Example of monodentate ethylenediamine.
B,HCl: [82888-77-5].
Orange solid. Sol. hot H_2O. Protonation occurs at the uncoordinated N.

Galsbol, F. *et al*, *Acta Chem. Scand., Ser. A*, 1982, **36**, 439 (*synth, uv, tga*)

$C_4H_{16}Cl_4N_4O_3Re_2$ IC-004360

Tetrachlorobis(ethylenediamine)trioxodirhenium(*V*)
Tetrachlorobis(1,2-ethanediamine-N,N′)-μ-oxodioxodirhenium(V), *9Cl*

[12547-48-7]



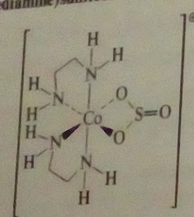
M 682.4
Linear OReOReO entity with octahedral coordination about Re. Synth. by reaction of Cl salt of Dioxobis(ethylenediamine)rhenium(*V*)(1+), IC-004378 in dil. aq. HCl. Green solid. Insol. Mp 195° dec. Ir $\nu_{Re=O}$ 980 cm^{-1}.

[35698-75-0]

Grove, D.E. *et al*, *J. Chem. Soc. A*, 1966, 1224 (*synth, ir, props*)
Glowiak, T. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1972, **20**, 199 (*cryst struct*)

$C_4H_{16}CoN_4O_3S^{\oplus}$ IC-004361

Bis(ethylenediamine)sulfitocobalt(*III*)(1+)

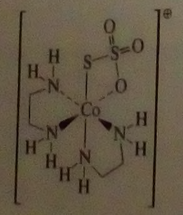


M 259.1 (ion)
Prob. octahedral struct.
Chloride: [17444-52-9].
Red-brown cryst. + $1H_2O$. Sol. H_2O.
Perchlorate: Orange-brown cryst. Sol. H_2O.
▷ Potentially explosive.

Baldwin, M.E. *et al*, *J. Chem. Soc.*, 1961, 3123 (*synth, uv, ir*)

$C_4H_{16}CoN_4O_3S_2^{\oplus}$ IC-004362

(Thiosulfato-*O,S*)bis(ethylenediamine)cobalt(*III*)(1+)
*Bis(1,2-ethanediamine-*N,N′*)[monothiosulfato(2−)-*O,S*]cobalt*(III)(*1+*), *10Cl*



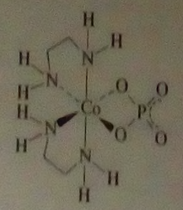
M 291.2 (ion)
Perchlorate: [74911-63-0].
Air-stable dark red solid. Sol. H_2O.
▷ Potentially explosive.

Cooper, J.N. *et al*, *Inorg. Chem.*, 1980, **19**, 3856 (*synth, ir, uv*)

$C_4H_{16}CoN_4O_4P$ IC-004363

Bis(ethylenediamine)phosphatocobalt(*III*)
*Bis(1,2-ethanediamine-*N,N′*)[phosphato(3−)-*O,O′*]cobalt*(III)

[19169-67-6]



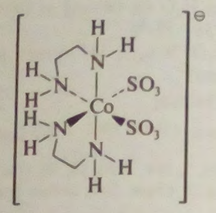
M 274.1
Mauve-red diamond-shaped plates.

Anderson, B. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 2652 (*cryst struct*)

$C_4H_{16}CoN_4O_6S_2^{\ominus}$ IC-004364

Bis(1,2-ethanediamine-*N,N′*)bis[sulfito(2−)-*S*]cobaltate(*III*)(1−), 10CI
Bis(ethylenediamine)disulfitocobaltate(III)(*1−*)

[62600-46-8]



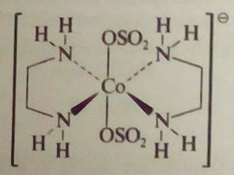
M 339.2 (ion)
cis-Octahedral anion with S-bonded sulfito groups.
Na salt: Yellow solid. Sol. H_2O.

[69823-39-8]

Baldwin, M.E., *J. Chem. Soc.*, 1961, 3123 (*synth, ir*)
Raston, C.L. *et al*, *Aust. J. Chem.*, 1979, **32**, 291 (*cryst struct*)

$C_4H_{16}CoN_4O_6S_2^{\ominus}$ IC-004365

Bis(1,2-ethanediamine-*N,N′*)bis(sulfito-*O*)cobaltate(1−), 9CI
Bis(ethylenediamine)disulfitocobaltate(III)(*1−*)



M 339.2 (ion)
Suitable anionic complex for kinetic studies.

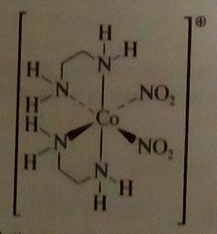
trans-form

Na salt: [29775-29-9].
Bright yellow cryst. + $3H_2O$.

Stranks, P.R., *Inorg. Chem.*, 1970, **9**, 751 (*kinetics*)
Inorg. Synth., 1973, **14**, 79 (*synth*)

$C_4H_{16}CoN_6O_4^{\oplus}$ IC-004366

Bis(ethylenediamine)dinitritocobalt(1+), 8CI
*Bis(1,2-ethanediamine-*N,N′*)bis(nitrito-*N*)cobalt*(*1+*), *9CI*
Dinitrobis(ethylenediamine)cobalt(III)(*1+*)



Absolute configuration

cis-Λ (−)-form

M 271.1 (ion)
Spontaneous resoln. occurs in *cis*-form on slow cryst. from H_2O.

cis-Λ(−)-form [18660-78-1]
Bromide: [15352-27-9].

Air-stable orange cryst. $[\alpha]_D$ −44° (0.5% H_2O in a 2-dm tube). Less sol. H_2O than racemate.

cis-Δ(+)-form [28074-44-4]
Bromide: [21350-93-6].
$[\alpha]_D$ +44°.
Chloride: [51321-44-9].

cis-(±)-form [20956-35-8]
Converts to *trans*-form on heating in soln.
Nitrite: Brown cryst.
Nitrate: Golden yellow needles (H_2O at <60°). Sol. H_2O (1.2 g per 100 cm^3 at 22°).

trans-form
Nitrate: [14240-12-1].
Air-stable, yellow cryst. (H_2O). Sol. H_2O (2.2 g per 100 cm^3 at 22°).
Iodide: [19636-81-8].
Cryst. Dec. at 209-218°.

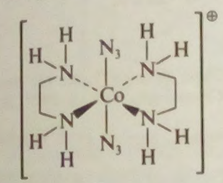
[42570-69-4]

Inorg. Synth., 1953, **4**, 176; 1960, **6**, 195; 1966, **8**, 196 (*synth, resoln*)
Bortin, O., *Acta Chem. Scand., Ser. A*, 1976, **30**, 503.
Bernal, I. *et al*, *Inorg. Chim. Acta*, 1985, **96**, 99; 1986, **122**, 213 (*synth, autoresoln, conformn, abs config, cryst struct*)

$C_4H_{16}CoN_{10}^{\oplus}$ IC-004367

Diazidobis(ethylenediamine)cobalt(*III*)(1+), 8CI
*Diazidobis(1,2-ethanediamine-*N,N′*)cobalt*(*1+*), *11CI, 10CI, 9CI*

[15489-32-4]



trans-form

M 263.1 (ion)
cis and *trans* isomers known. *cis*-form is optically active and has been resolved.

cis-form [24996-37-0]
Distorted octahedral config. about Co with linear N_3 groups. Co—NN 197; Co—NC 200 pm. Salts are red.
Chloride: [68265-39-4].
Red.
Bromide: [15275-20-4].
Red cryst. Ir δ_{N_3} 677, 657 cm^{-1} (nujol).
Iodide: [79270-30-7].
Cryst.
Perchlorate: [14877-87-3].
Dark red cryst. Ir ν_{N_3} 2075, 2028 cm^{-1} (nujol).
Nitrate: [22651-44-1].
Deep red cryst. Ir ν_{N_3} 2024, 2022 cm^{-1} (nujol).
Azide: [42863-01-4].
Synth. in 1:1 mixt. with *trans* isomer. Cryst.

cis-Δ-form [39502-33-5]
$(+)_D$-cis-*form*
Kindred *et al* dispute this assignment, and propose that Λ is the $(+)_D$ form.
Perchlorate: [61542-81-2].
Red-violet fine cryst. (H_2O). $[\alpha]_D$ +237° ; $[\alpha]_{546}$ −962°.

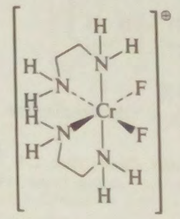
cis-Λ-form [56906-68-4]
$(-)_D$-cis-*form*
Perchlorate: Cryst. (hot H_2O). $[\alpha]_+$°, −237; $[\alpha]_{546}$ +962°.

trans-form [24996-36-9]
Salts are purple.
Perchlorate: [14781-34-1].
Brown-purple cryst. Ir ν_{N_3} 2020 cm^{-1} (nujol).
Azide: [42863-02-5].
Synth. in 1:1 mixt. with *cis* isomer. Cryst.

Staples, P.J. *et al*, *J. Chem. Soc.*, 1960, 4812 (*cis, trans, salts, synth, ir, uv-vis, resoln*)
Lantzke, I.R. *et al*, *Aust. J. Chem.*, 1967, **20**, 35 (*pmr*)
Buckingham, D.A. *et al*, *Aust. J. Chem.*, 1967, **20**, 257 (*pmr*)
Padmanabhan, V.M. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 1638 (*cryst struct, cis-nitrate*)
Druding, L.F. *et al*, *J. Coord. Chem.*, 1973, **3**, 105 (*ir, pmr*)
Kindred, I.J. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 1359 (*cd, abs config*)
Yamasaki, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 3060 (*cd, abs config, resoln, uv-vis*)
Jackson, W.G. *et al*, *Inorg. Chem.*, 1984, **23**, 659 (*base hydrol*)

$C_4H_{16}CrF_2N_4^{\oplus}$ IC-004368

Bis(ethylenediamine)difluorochromium(*III*)(1+), 8CI
*Bis(1,2-ethanediamine-*N,N′*)difluorochromium*(*1+*), *11CI, 10CI, 9CI*



cis-form

M 210.1 (ion)
Octahedral anion.

cis-form [22432-37-7]
Iodide: [15444-78-7].
Starting material for compds. *cis*-$[Cr(en)_2FX]I$, X = $Cl^{\ominus}$, $Br^{\ominus}$, $NCS^{\ominus}$, H_2O, NH_3. Pink solid + H_2O (aq. HI/EtOH). More sol. than *trans*-complex. This salt has been resolved into its Λ and Δ forms.
Perchlorate: [59765-96-7].
Synth. from *cis*-$[Cr(en)_2F_2][Cr(en)F_4]$ + 6*M* $HClO_4$ and H_2O. Solid. Sol. H_2O.
(*Ethylenediamine*)*tetrafluorochromate*(III) *salt:* see (*Ethylenediamine*)*tetrafluorochromate*(III)(*1−*), *IC-003290*

trans-form [24407-74-7]
Chloride: [19581-00-1].
Synth. from $CrCl_3.6H_2O$, HF and aq. ethylenediamine. Orange red cryst. (H_2O). Sol. H_2O.
Perchlorate: [19581-04-5].
Synth. from *trans*-$[CrPy_4F_2]ClO_4$ and ethylenediamine heated under reflux. Bright red cryst. (H_2O or 0.1*M* $HClO_4$).
Bromide: [19581-01-2].
Red(?) cryst. (H_2O). Sol. H_2O.

[14588-00-2, 26318-81-0, 42281-18-5, 69926-04-1]

Vaughn, J.W. *et al*, *Inorg. Chem.*, 1968, **7**, 736; 1979, **18**, 1509 (*resoln, cis-form, synth, trans salt*)
Glerup, J. *et al*, *Acta Chem. Scand.*, 1970, **24**, 247 (*synth, trans-form, perchlorate*)
Garner, C.S., *Adv. Transition Met. Chem.*, 1970, **6**, 97 (*rev*)
Brencic, J.V. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **480**, 213 (*cryst struct, trans-form*)
Inorg. Synth., 1986, **24**, 185 (*cis salts*)

IC-004369

$C_4H_{16}CrN_4O_4S$
Bis(ethylenediamine)sulfatochromium(*II*), 8CI

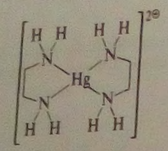
$Cr(SO_4)(H_2NCH_2CH_2NH_2)_2$

M 268.2
6-Coordinate through *trans* bridging anions. Violet air-sensitive solid. Sol. H_2O. $\mu_{eff} = 4.80\mu_B$ (300K); $4.56\mu_B$ (90K).

Larkworthy, L.F. *et al*, *J. Chem. Soc. A*, 1969, 1339 (*synth, props*)

IC-004370

$C_4H_{16}HgN_4^{2\oplus}$
Bis(ethylenediamine)mercury(2+)
Bis(1,2-ethanediamine-N,N′)mercury(2+)
[40712-15-0]



M 320.7 (ion)
Diperchlorate: [60111-90-2].
Prepd. from $Hg(ClO_4)_2$ + ethylenediamine. Colourless cryst. (H_2O).

Pfeiffer, P. *et al*, *Z. Anorg. Allg. Chem.*, 1952, **270**, 287 (*synth*)
Duplancic, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 887 (*cryst struct*)

IC-004371

$C_4H_{16}HgN_8S_4^{2\oplus}$
Tetrakis(thiourea-*S*)mercury(2+)
[23190-59-2]

$[Hg[S{=}C(NH_2)_2]_4]^{2\oplus}$

M 505.0 (ion)
Tetrahedral cation: H-bonding between thiourea groups and counteranion.
Dichloride: [2881-22-1]. *Dichlorotetrakis(thiourea-S)mercury(II). Mercury(II) chloride tetrakis (thiourea)*
Cryst. (H_2O). Mp 140°. Dec. at 183°.
Dibromide:
$C_4H_{16}Br_2HgN_8S_4$ M 664.8
Cryst. Mp 157°
Diiodide:
$C_4H_{16}HgI_2N_8S_4$ M 758.8
Cryst. Mp 95°
Bis-tetrafluoroborate: [40780-37-8].
Cryst. (H_2O).
Diperchlorate: [40793-08-6].
Cryst. (H_2O)
Dinitrate: [26920-94-5]. *Dinitratotetrakis(thiourea)mercury*
Cryst.
Sulfate: [20249-77-8].
Cryst. Forms a monohydrate.

[13695-44-0, 20631-51-0, 33887-28-4]

Inorg. Synth., 1960, **6**, 26 (*synth*)
Czako-Sulikowska, D.M. *et al*, *Pol. J. Chem. (Rocz. Chem.)*, 1967, **41**, 843; 1969, **43**, 1353 (*synth, ir*)
Ashcroft, S.J. *et al*, *J. Chem. Soc. A*, 1970, 1020 (*heat of formn*)
Korczynski, A. *et al*, *Cryst. Struct. Commun.*, 1972, **1**, 327 (*cryst struct, chloride*)
Brotherton, P.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2696 (*cryst struct, chloride*)
Peyronel, G. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1117 (*synth*)

IC-004372

$C_4H_{16}IN_5ORu^{2\oplus}$
Bis(ethylenediamine)iodo(nitrosyl)ruthenium(2+)
Bis(1,2-ethanediamine-N,N′)iodo(nitrosyl)ruthenium(2+)

$[Ru(NO)I(NH_2CH_2CH_2NH_2)_2]^{2\oplus}$

M 378.1 (ion)
Reported in early literature; struct. unknown.
Diodide salt:
$C_4H_{16}I_3N_5ORu$ M 631.9

Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 242 (*synth*)

IC-004373

$C_4H_{16}I_2N_4Pt^{2\oplus}$
Bis(ethylenediamine)diiodoplatinum(*IV*), 8CI
Bis(1,2-ethanediamine-N,N′)diiodoplatinum(2+), 10CI
[19184-31-7]
As Dibromobis(ethylenediamine)platinum(*IV*), IC-004330 with

X = I

M 569.0 (ion)
trans-isomer most studied. Forms many double salts with square planar $M^{2\oplus}$ ions having stacked structs. and one-dimensional electrical conductance.
Diiodide: [79019-30-0].
$C_4H_{16}I_4N_4Pt$ M 822.8
Golden needles or plates + $2H_2O$.
Bis(ethylenediamine)platinum(2+) double salt, tetraperchlorate: [62535-09-5].
$C_8H_{32}Cl_4I_2N_8O_{16}Pt_2$ M 1282.1
Dark red prisms.

[87525-32-4]

Bekaroglu, O. *et al*, *Inorg. Chim. Acta*, 1977, **21**, 183 (*synth*)
Matsumoto, N. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 1458 (*cryst struct*)
Endres, H. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 1885 (*cryst struct*)
Freckmann, B. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 1520 (*synth, cryst struct*)
Clark, R.J.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 524 (*ir, raman, uv-vis*)
Aoki, R. *et al*, *Mol. Cryst. Liq. Cryst.*, 1982, **81**, 301 (*esr, elec cond*)

IC-004374

$C_4H_{16}I_2N_4Ru^{\oplus}$
Bis(ethylenediamine)diiodoruthenium(*III*)(1+)
Bis(1,2-ethanediamine-N,N′)diiodoruthenium(1+), 9CI.
Bis(1,2-diaminoethane)diiodoruthenium(III)*(1+)*
As Dibromobis(ethylenediamine)ruthenium(*III*)(1+), IC-004332 with

X = I

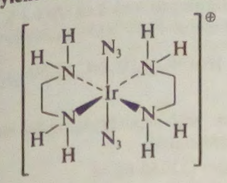
M 475.0 (ion)
The cation is readily hydrated for both isomers. Sol. H_2O.
cis-form [45839-24-5]
(Ethylenediamine)tetraiodoruthenate(1−) salt: [15406-29-8].
$C_8H_{24}I_8N_8Ru_2$ M 1143.8
Prepd. by treating [Ru(en)-(oxalato)$^{\oplus}$][Ru(en)$(oxalato)_2^{\ominus}$] with aq. HI. Dark green solid. μ_{eff} = $1.99\mu_B$ (per Ru atom).
trans-form [87655-42-3]
Prepd. by heating the *trans*-form of Dichlorobis(ethylenediamine)ruthenium(1+), IC-004357 with an excess of NaI.

Broomhead, J.A. *et al*, *J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, magnetism*)

Poon, C.-K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 756; 1982, 531 (*synth, photochem*)
Poon, C.-K. *et al*, *Inorg. Chem.*, 1983, **22**, 3893; 1984, **23**, 2130 (*equation, uv, reactions, electron transfer*)

IC-004375

$C_4H_{16}IrN_{10}^{\oplus}$
Diazidobis(ethylenediamine)iridium(*III*)(1+), 8CI

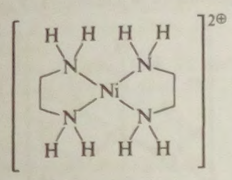


M 396.4 (ion)
trans-form known only.
Hexafluorophosphate: [26104-26-7].
Yellow cryst.

Bauer, B.A. *et al*, *Inorg. Chem.*, 1969, **8**, 2231 (*synth, uv*)

IC-004376

$C_4H_{16}N_4Ni^{2\oplus}$
Bis(ethylenediamine)nickel(*II*)(2+), 8CI
Bis(1,2-ethanediamine-N,N′)nickel(II)*(2+), 9CI. Bis(1,2-diaminoethane)nickel*(II)*(2+)*
[15390-98-4]



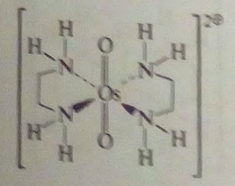
M 178.8 (ion)
Much studied square planar complex. Occurs with anions which are poor ligands. Some examples are thermochromic: blue ⇌ yellow.
Diperchlorate: [15747-95-2].
$C_4H_{16}Cl_2N_4NiO_8$ M 377.7
Yellow solid.
▷ Potentially explosive.
Bis-dibromoargentate(1−): [16040-59-8].
$C_4H_{16}Ag_2Br_4N_4Ni$ M 714.2
Isomorphous with $AgI_2^{\ominus}$ salt with square planar Ni ions and $[AgBr]_n^{n\ominus}$ chains. Orange cryst.
Bis-diiodoargentate(1−): [23105-69-3].
$C_4H_{16}Ag_2I_4N_4Ni$ M 902.2
Orange cryst.

[42534-33-8]

Sone, K. *et al*, *Z. Anorg. Allg. Chem.*, 1959, **301**, 277 (*synth, uv*)
Lever, A.B.P. *et al*, *J. Chem. Soc.*, 1963, 2552 (*synth, ir, uv*)
Stomberg, R., *Acta Chem. Scand.*, 1969, **23**, 3498 (*cryst struct*)

IC-004377

$C_4H_{16}N_4O_2Os^{2\ominus}$
Bis(ethylenediamine)dioxoosmium(*IV*)(2+)
Bis(1,2-ethanediamine-N,N′)dioxoosmium(IV)*(2+)*
[61202-82-2]

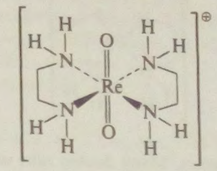


M 342.3 (ion)
Dichloride: [65468-15-7].
Synth. from $K_2[OsO_4(OH)_4]$ and en.2HCl. Dull yellow-orange solid.
Bis(hydrogen sulfate): [61202-83-3].
Obt. by metathesis of corresp. dichloride with H_2SO_4. Monoclinic cryst.

Malin, J.M. *et al*, *Inorg. Chem.*, 1971, **10**, 2403; 1977, **16**, 615 (*synth, ir, cryst struct*)
Murman, R.K., *J. Inorg. Nucl. Chem.*, 1977, **39**, 1317 (*use, uv, ir*)
Habron, S.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 633 (*pmr, use*)

IC-004378

$C_4H_{16}N_4O_2Re^{\oplus}$
Dioxobis(ethylenediamine)rhenium(*V*)(1+)
Bis(1,2-ethanediamine-N,N′)dioxorhenium(V)*(1+), 9CI*
[21602-78-8]



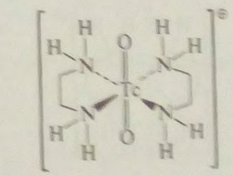
M 338.4 (ion)
Octahedral.
trans-form
Interatomic distances: Re=O ~ 179, 176, Re—N ~ 215.4, 215.0 pm.
Chloride: [14405-69-7].
Synth. from K_2ReCl_6, en, and H_2O in air. Brownish green cryst. (aq. MeOH).
Perchlorate: Synth. from the chloride and $HClO_4$ aq. Purple cryst.
▷ Potentially explosive.

[14587-92-9]

Inorg. Synth., 1966, **8**, 173 (*synth*)
Sergienko, V.S. *et al*, *Zh. Strukt. Khim.*, 1974, **15**, 275 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1636 (*synth*)
Lock, C.J.L. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 923 (*cryst struct*)

IC-004379

$C_4H_{16}N_4O_2Tc^{\oplus}$
Bis(ethylenediamine)dioxotechnetium(*V*)(1+)
Bis(1,2-ethanediamine-N,N′)dioxotechnetium(V)*(1+), 11CI*
[84204-58-0]



M 251.1 (ion)
trans-Octahedral cation. The chelate rings are *δλ* in the $I^{\ominus}$ salt, but the $Cl^{\ominus}$ salt contains both *δδ* and *λλ* configurations. Synth. from $TcOCl_4^{\ominus}$ plus ligand in THF, from Tc-citrate species + ligand, or by Sn(*II*) redn. of $TcO_4^{\ominus}$ + ligand.
Chloride: [37473-42-0].
Orange needles. Diamagnetic.
Iodide: [80720-95-2].
Yellow plates. Spar. sol. H_2O.

Dyrssdsen, J.S. *et al. Ibr. J. Appl. Radiat. Isot.*, 1965, **16**, 633 (synth, analysis)
Knetsch, M.E. *et al. Inorg. Chem.*, 1982, **21**, 3047 (synth, cryst struc, ir, uv)
Johansson, K. *Ibr. J. Appl. Radiat. Isot.*, 1980, **31**, 429 (spectr, synthesis)
Vinkler, M.A. *et al. Ibr. J. Appl. Radiat. Isot.*, 1980, **31**, 691 (synth, analysis)
Hoffman, T.J. *et al. Ibr. J. Appl. Radiat. Isot.*, 1980, **31**, 225 (synth, analysis)
Soldini, G. *et al. Appl. Radiat. Isot.*, 1980, **40**, 637 (spectrum, coupl, analysis)

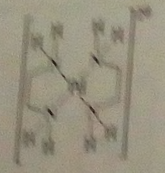
IC-004380

$C_2H_{10}N_4Pd^{2\oplus}$

Bis(ethylenediamine)palladium(*II*)(2+), 8Cl

Bis(1,2-ethanediamine-N,N′)palladium(II)(2+), 8Cl

[23578-09-6]



M 228.6 (ion)
Square planar struct. Many double salts with $M(II)$ cations, giving stacked polymeric structs.

Dichloride: [14063-35-6]
$C_4H_{18}Cl_2N_4Pd$ M 307.5
Colourless prisms. Sol. H_2O.

Dipicrolonate, double salt with dichloro(bis(ethylenediamine) palladium) 4-oxopicrolonate: [67025-21-2].
Stacked struct. with Pd^{2+}—Cl 303, Pd^{4+}—Cl 252 pm.

Drew, H.D.K. *et al. J. Chem. Soc.*, 1932, 1895 (*synth*)
Baggio, S. *et al. Acta Crystallogr., Sect. B*, 1970, **26**, 1609 (*cryst struct*)
Appleton, T.G. *et al. Inorg. Chem.*, 1970, **9**, 1807 (*pmr*)
Papaconstantinou, G.C. *et al. J. Chem. Soc., Faraday Trans. 2*, 1981, **77**, 581 (*double salts*)
Banerjeaee, A.L. *et al. Acta Crystallogr., Sect. B*, 1982, **38**, 1158 (*double salts*)
Nakiyama, K. *et al. Bull. Chem. Soc. Jpn.*, 1984, **57**, 2850 (*uv, mol*)

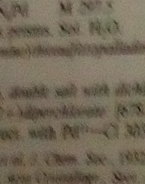
IC-004381

$C_4H_{16}N_4Pt^{2\oplus}$

Bis(ethylenediamine)platinum(*II*)(2+), 8Cl

Bis(1,2-ethanediamine-N,N′)platinum(2+)

[19184-30-6]



M 315.2 (ion)
Simplest bis-diamine $Pt(II)$ complex. Widely studied. Many salts are known including double salts with other metal cations, including $Pt(IV)$ species.

Dichloride: [15352-47-3].
$C_4H_{16}Cl_2N_4Pt$ M 386.1
Commercially available. White solid. Sol. H_2O.

Diperchlorate: [28136-92-7].
Pale cream solid. Sol. H_2O, MeCN.
▷ Potentially explosive.

Basolo, F. *et al. J. Am. Chem. Soc.*, 1950, **72**, 2433 (*synth*)
Mizuno, K.A. *et al. J. Inorg. Nucl. Chem.*, 1973, **34**, 275 (*synth*)
Berg, R.W. *et al. Spectrochim. Acta, Part A*, 1972, **28**, 2319 (*ir, cation*)
Mason, W.R., *Inorg. Chem.*, 1986, **25**, 2025 (*uv-vis, mcd*)

IC-004382

$C_2H_{10}N_6NiO_2^{\oplus}$

Bis(ethylenediamine)nitronickel(*II*)(1+), 8Cl

Bis(1,2-ethanediamine-N,N′)nitronickel(1+), 9Cl

$[Ni(NO_2)_2(H_2NC_2H_4NH_2)_2]^{\oplus}$

M 224.8 (ion)
Polymeric struct. with *N,O* bridging by $NO_2^{\ominus}$; counter anions uncoordinated.

Tetrafluoroborate: [32032-63-6].
Red cryst.

Perchlorate: [50409-58-9].
Orthorhombic red cryst.
▷ Potentially explosive.

[66767-65-9]

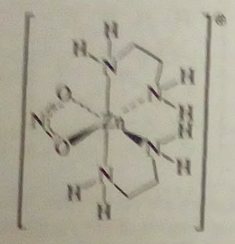
Finney, A.J. *et al. Aust. J. Chem.*, 1981, **34**, 2159 (*cryst struct*)
Meyer, A. *et al. Inorg. Chem.*, 1982, **21**, 1729 (*synth, magnetism, cryst struct*)

IC-004383

$C_4H_{16}N_6O_2Zn^{\oplus}$

Bis(ethylenediamine)(nitrito)zinc(1+)

Bis(1,2-ethanediamine-N,N′)(nitrito-O,O′)zinc(1+), 9Cl



M 231.5 (ion)
Approx. octahedral at Zn.

Bromide: [52620-67-4].
Cryst. (H_2O).

Nitrite: [80582-58-7].
Cryst. (EtOH/Et_2O or H_2O).

Perchlorate: [81174-45-0].
Cryst. (H_2O).
▷ Potentially explosive.

[52620-66-3, 52665-55-0, 80582-61-2]

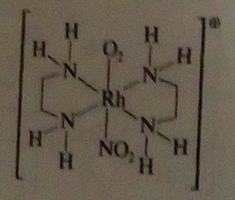
Goodgame, D.M.L. *et al. J. Chem. Soc. A*, 1970, 1933 (*synth, ir*)
Sveiashvili, A.E. *et al. J. Struct. Chem. USSR (Engl. Transl.)*, 1974, **15**, 284 (*synth, cryst struct*)
Sveiashvili, A.E., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 307 (*synth*)
Finney, A.J. *et al, Aust. J. Chem.*, 1981, **34**, 2061, 2159 (*cryst struct, nitrite salt, ir*)

IC-004384

$C_4H_{16}N_6O_4Rh^{\oplus}$

Bis(ethylenediamine)nitritohyperoxyrhodium(*III*), 10Cl

Bis(ethylenediamine)nitrosuperoxorhodium(III)



M 301.1 (ion)
Chloride: [63128-76-7].
Red solid.
(*nitrato, R.D. et al, J. Chem. Soc., Chem. Commun.*, 1973, 58 (*synth, str, raman*)

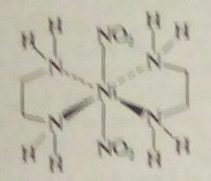
IC-004385

$C_2H_{10}N_6NiO_4$

Bis(ethylenediamine)dinitronickel(*II*)

Bis(1,2-ethanediamine-N,N′)bis(nitrito-N)nickel(II), 9Cl

[14521-87-0]



M 270.8
Octahedral complex.

rans-form [17835-68-6]
Red cryst. (MeOH); isom. to blue dinitrito, probably *O*-bonded, compsl. on heating.

[52049-78-2, 53195-52-1]

Goodgame, D.M.L. *et al, Inorg. Chem.*, 1966, **5**, 1303 (*synth, ir, spectra*)
Green, R.W., *Aust. J. Chem.*, 1973, **26**, 1841 (*isom*)
Sveiashvili, A.C. *et al, Zh. Strukt. Khim.*, 1974, **15**, 307 (*synth, cryst struct, cis-form*)
Finney, A.J. *et al, Aust. J. Chem.*, 1981, **34**, 2047 (*cryst struct, ir*)
Shakhishneider, T. *et al, J. Therm. Anal.*, 1987, **33**, 525 (*isom*)

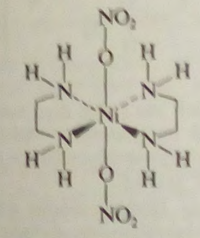
IC-004386

$C_2H_{10}N_6NiO_6$

Bis(ethylenediamine)dinitratonickel(*II*)

Bis(1,2-ethanediamine-N,N′)bis(nitrato-O)nickel(II), 9Cl.
Nickel(II) nitrate bis(ethylenediamine)

[14639-34-0]



M 302.8
Has monodentate $NO_3^{\ominus}$ ligands. Octahedral, assumed *trans* config. Green-blue solid. Ir ν_{N1-N} 380s 295.5m cm^{-1} (nujol). Paramagnetic.

[42590-60-3]

Curtis, N.F. *et al, Inorg. Chem.*, 1965, **4**, 804.
Lever, A.B.P. *et al, Can. J. Chem.*, 1973, **51**, 1567 (*ir*)

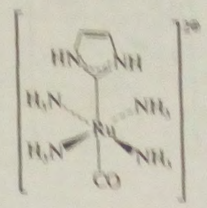
IC-004387

$C_4H_{16}N_6ORu^{2\oplus}$

Tetraamminecarbonyl(1,3-dihydro-2*H*-imidazol-2-ylidene) ruthenium(*II*)(2+), 9Cl

Tetraammine(carbonyl)(imidazole)ruthenium(II)(2+)

[81872-15-3]



M 265.2 (ion)
The imidazole ligand is bound through C(2) as an ylid; *trans*-octahedral. Prepd. by reducing Tetraamminechloro(1,3-dihydro-2*H*-imidazol-2-ylidene) ruthenium(2+), IC-003740 with Zn/Hg, followed by CO. Sol. H_2O.

Bis-hexafluorophosphate

[52124-95-7]

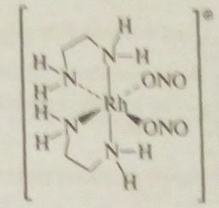
Sundberg, R.J. *et al, J. Am. Chem. Soc.*, 1974, **96**, 381 (*synth, pmr, uv, electrochem*)
Tweedle, M.F. *et al, Inorg. Chem.*, 1982, **21**, 3361 (*isomerization, reaction, electrochem*)

IC-004388

$C_4H_{16}N_6O_4Rh^{\oplus}$

Bis(ethylenediamine)dinitritorhodium(*III*)(1+)

Bis(1,2-ethanediamine-N,N′)bis(nitrito-O)rhodium(III)(1+)



cis-form

M 315.1 (ion)
Octahedral.

cis-form

Nitrate: White needles.

trans-form

Nitrate: White cryst.

Johnson, S.A. *et al, Inorg. Chem.*, 1962, **1**, 925 (*synth, ir, uv*)

IC-004389

$C_4H_{16}N_8O_5S_5V$

Oxo[sulfato(2−)-*O,O′*]tetrakis(thiourea-*N*)vanadium(*IV*), 1ICl

[88667-77-0]

$VO(SO_4)[S{=}C(NH_2)_2]_4$

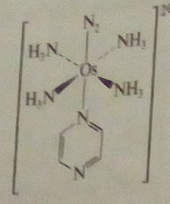
M 467.4
Synth. heating under reflux $VOSO_4 \cdot 2H_2O$ and thiourea in EtOH. Blue solid. Mp 120°. Paramagnetic, μ_{eff} = $2.44\mu_B$, g = 2.011.

Adi, M.B. *et al, J. Indian Chem. Soc.*, 1983, **60**, 729 (*synth, uv-vis, ir, magnetism*)

$C_4H_{16}N_8Os^{2\oplus}$ IC-004390

Tetraammine(dinitrogen)pyrazineosmium(*II*)(2+)

[84711-81-9]



M 366.4 (ion)

trans-Octahedral.

Dibromide: [57253-54-0].

Synth. from an aq. soln. of bis(dinitrogen) tetraammineosmium(*II*)chloride and excess pyrazine, followed by evap. and metathesis with NaBr. Red-orange solid. Ir ν_{N-N} 2040 cm^{-1}.

Magnuson, R.H. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 5129 (*synth, ir, uv*)

Johnson, C. *et al*, *Inorg. Chem.*, 1983, **22**, 1117 (*uv, pKa*)

$C_4H_{16}N_8PbS_4^{2\oplus}$ IC-004391

Tetrakis(thiourea)lead(*II*)(2+)

[32326-81-1]

$[Pb[S{=}C(NH_2)_2]_4]^{2\oplus}$

M 511.6 (ion)

Diperchlorate: [16774-39-3]. *Lead*(II) *perchlorate tetrakis(thiourea)*

Obt. from $Pb(ClO_4)_2$ and thiourea. Pale yellow needles.

▷ Potentially explosive.

Dipicrate: [9072-70-2].

Obt. by slow cooling of an aq. soln. containing thiourea and lead picrate. Mp 159° dec.

▷ Potentially explosive.

Swaminathan, K. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 1291 (*synth, ir, perchlorate*)

Adams, D.M. *et al*, *J. Chem. Soc. A*, 1967, 884 (*far-ir*)

Herbstein, F.H. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 405 (*cryst struct, picrate*)

$C_4H_{16}N_8PdS_4^{2\oplus}$ IC-004392

Tetrakis(thiourea)palladium(*II*)(2+)

[42941-76-4]

$[[(H_2N)_2C{=}S]_4Pd]^{2\oplus}$

M 410.9 (ion)

Dichloride: [14587-98-5].

$C_4H_{16}Cl_2N_8PdS_4$ M 481.8

Bright red needles (H_2O). Exists in 2 crystalline forms.

Bis-tetraphenylborate: [20774-42-9].

Yellow solid. Mp 180-181°.

[53637-86-8, 53637-87-9]

Yamaguchi, A. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 527 (*synth, ir*)

Ooi, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1960, **33**, 861 (*cryst struct, chloride*)

Tarantelli, T. *et al*, *J. Chem. Soc. A*, 1968, 1717 (*synth*)

Berta, D.A., *Inorg. Chem.*, 1970, **9**, 136 (*cryst struct, chloride*)

Kharitonov, Yu.Ya., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 1187 (*ir*)

$C_4H_{16}N_8PtS_4^{2\oplus}$ IC-004393

Tetrakis(thiourea)platinum(*II*)(2+), 8CI

[48069-54-1]

$Pt[SC(NH_2)_2]_4^{2\oplus}$

M 499.5 (ion)

Square planar struct. Formed from *cis*-$[Pt(NH_3)_2X_2]$ (X = halide) but not *trans*-isomer (Kurnakov's test).

Di-Chloride: [14552-88-6].

$C_4H_{16}Cl_2N_8PtS_4$ M 570.4

Yellow needles. Sol. H_2O.

Hexachloroplatinate(2−): [18793-69-6].

$C_4H_{16}Cl_6N_8Pt_2S_4$ M 907.3

Orange-red microcryst. Shows mixed valence transitions.

Kurnakov, N., *J. Prakt. Chem.*, 1894, **50**, 485 (*synth*)

Girling, R.L. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 557 (*cryst struct*)

Kharitonov, Yu.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 1187 (*ir*)

Arrizabalaga, P. *et al*, *Chem. Phys. Lett.*, 1980, **76**, 548 (*uv-vis, pe, Pt-195 nmr*)

Bret, J.M. *et al*, *Inorg. Chim. Acta*, 1981, **51**, 103 (*synth, pe*)

Woollins, J.D. *et al*, *Polyhedron*, 1983, **2**, 175 (*pmr, cmr, Pt-195 nmr*)

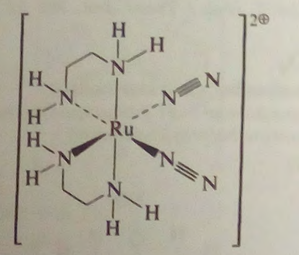
$C_4H_{16}N_8Ru^{2\oplus}$ IC-004394

Bis(dinitrogen)bis(ethylenediamine)ruthenium(*II*)(2+)

Bis(1,2-diaminoethane)bis(dinitrogen)ruthenium(II).

*Bis(dinitrogen)bis(1,2-ethanediamine-*N,N′*)ruthenium*(2+), *9CI*

[46136-63-4]



M 277.2 (ion)

cis-Octahedral. Much less stable than mono(dinitrogen) analogues. Prepd. by treating *cis*- Azido(dinitrogen) bis(ethylenediamine)ruthenium(*II*)(1+), IC-004397 with nitrous acid at 0° rapidly.

Bis-tetraphenylborate: Highly unstable solid, contaminated with Aqua(dinitrogen)(ethylenediamine)ruthenium(*II*)(2+), IC-004423. Ir ν_{N_2} 2220, 2190 cm^{-1}. Dec. in *ca.* 30 minutes.

Kane-Maguire, L.A.P. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5295; 1970, **92**, 5865 (*synth, ir, dec*)

$C_4H_{16}N_8S_4Zn^{2\oplus}$ IC-004395

Tetrakis(thiourea-*S*)zinc(2+)

$Zn[S{=}C(NH_2)_2]_4^{2\oplus}$

M 369.8 (ion)

Dichloride: [28813-20-9]. *Dichlorotetrakis(thiourea-*S*)zinc*(II)

Cryst. Mp 222°. Dec. at 228°.

Dinitrate: [19596-79-3]. *Zinc*(II) *nitrate tetrakis(thiourea)*

$C_4H_{16}N_{10}O_6S_4Zn$ M 493.8

White non-hygroscopic prisms (H_2O). Mp 92°. Dec. above Mp. eventually to ZnS.

Diperchlorate: [19596-77-1]. *Zinc*(II) *perchlorate tetrakis(thiourea)*

Cryst. Mp 116°.

▷ Potentially explosive.

Bis-tetrafluoroborate: [40793-00-8].

$C_4H_{16}B_2F_8N_8S_4Zn$ M 543.4

Cryst.

Sulfate: [33887-28-4]. *Sulfatotetrakis(thiourea)zinc*(II)

$C_4H_{16}N_8O_4S_5Zn$

Cryst. Mp 200°. Dec. at 240°.

[23862-08-0]

Flint, C.D. *et al*, *J. Chem. Soc. A*, 1967, 1718 (*synth, ir*)

Ashcroft, S.J. *et al*, *J. Chem. Soc. A*, 1970, 1020.

Protsenko, P.I. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1971, **16**, 1748 (*synth*)

Peyronel, G. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1117 (*synth, stability const*)

Molchanov, Ya.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 1247 (*synth*)

Eaton, D.R., *J. Inorg. Nucl. Chem.*, 1976, **38**, 1007 (*pmr*)

Vega, R. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 2297 (*cryst struct*)

Eaton, D.R., *Inorg. Chem.*, 1980, **19**, 740 (*synth*)

Dremyatskaya, L.D. *et al*, *Zh. Fiz. Khim.*, 1969, **43**, 850 (*ir*)

Geroleva, O.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 780 (*synth*)

Pino Aransibia, J.I. *et al*, *Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1977, **20**, 301; *CA*, **86**, 198281 (*cryst struct*)

$C_4H_{16}N_8Se_4Zn^{2\oplus}$ IC-004396

Tetrakis(selenourea-*Se*)zinc(2+)

$[Zn[Se{=}C(NH_2)_2]_4]^{2\oplus}$

M 557.4 (ion)

Dinitrate: [38901-20-1]. *Zinc nitrate tetrakis-selenourea*

Cryst. Insol. C_6H_6, Et_2O.

Diperchlorate: [38901-19-8]. *Zinc perchlorate tetrakis-selenourea*

Cryst. Insol. C_6H_6, Et_2O.

Sulfate: [38643-67-3]. *Tetrakis(selenourea-*Se*)zinc(2+) sulfate. Zinc sulfate tetrakis-selenourea*

Cryst.

Aitken, G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 2103 (*synth, ir*)

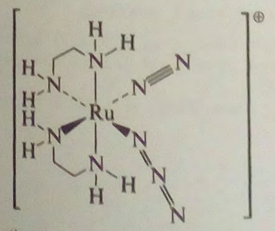
Usbalieva, U. *et al*, *Zh. Neorg. Khim.*, 1974, **19**, 1652 (*synth*)

Udupa, M.R. *et al*, *J. Indian Chem. Soc.*, 1972, **49**, 775 (*synth, ir*)

$C_4H_{16}N_9Ru^{\oplus}$ IC-004397

Azido(dinitrogen)bis(ethylenediamine)ruthenium(*II*)(1+)

*Azido(dinitrogen)bis(1,2-ethanediamine-*N,N′*)ruthenium*(1+). *Azidobis(1,2-diaminoethane)(dinitrogen)ruthenium*(II)(1+)



cis-form

M 291.3 (ion)

Pseudo-octahedral.

cis-form [46240-14-6]

Prepd. by *cis*-Diazidobis(ethylenediamine) ruthenium(1+), IC-004399 at 65° for 30 min.

Hexafluorophosphate: Brown diamagnetic powder, stored in the dark at −15° to prevent loss of N_2. Ir ν_{N_2} 2130; ν_{N_3} 2050 cm^{-1}.

trans-form [46240-13-5]

N≡N 110.6; RuN—N_2 117.9; RuN_2—N 114.6; Ru—N_2 189.4; Ru—N_3 212.1; Ru—N_{en} 212.5 pm; angles, Ru—N≡N 179°; Ru—N=NN 117°. Prepd. by gently heating *trans* Diazidobis(ethylenediamine) ruthenium(1+), IC-004399.

Hexafluorophosphate: Solid. Ir ν_{N_2} 2103 cm^{-1}.

[46240-12-4]

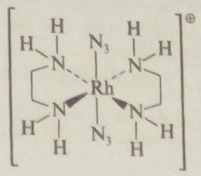
Kane-Maguire, L.A.P. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5295; 1970, **92**, 5865 (*synth, reaction*)

Davis, B.R. *et al*, *Inorg. Chem.*, 1970, **9**, 2768 (*synth, cryst struct, ir*)

Kane-Maguire, L.A.P., *J. Inorg. Nucl. Chem.*, 1971, **33**, 3964 (*synth, ir, reactions*)

$C_4H_{16}N_{10}Rh^{\oplus}$ IC-004398

Diazidobis(ethylenediamine)rhodium(*III*)(1+)



trans-form

M 307.1 (ion)

trans-form

Chloride: Deep golden cryst. solid, turning brown in sunlight after several hours. Sol. H_2O.

Johnson, S.A. *et al*, *Inorg. Chem.*, 1962, **1**, 925.

$C_4H_{16}N_{10}Ru^{\oplus}$ IC-004399

Diazidobis(ethylenediamine)ruthenium(1+)

*Diazidobis(1,2-ethanediamine-*N,N′*)ruthenium*(1+), *9CI*. *Bis(azido)bis(1,2-diaminoethane)ruthenium*(III)

[4361-42-6]

As Dichlorobis(ethylenediamine)ruthenium(1+), IC-004357 with

X = N_3

M 305.3 (ion)

cis-Octahedral; can be prepd. optically pure. Dec. both in soln. and in the solid state to evolve N_2, prob. via a nitrene intermed.

Hexafluorophosphate: Prepd. by treating Dichlorobis(ethylenediamine)ruthenium(1+), IC-004357 with $Ag^{\oplus}$, followed by $[N_3]^{\ominus}$ and $[PF_6]^{\ominus}$. Deep purple-red cryst. May be stored as a solid for several weeks, if kept at −15° in the dark. μ_{eff} = 2.0μ_B; Ir ν_{N_3} 2050 cm^{-1}.

[4361-41-5]

Inorg. Synth., 1970, **12**, 23 (*synth*)

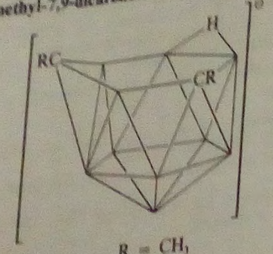
Kane-Maguire, L.A.P. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 5865 (*synth, ir, uv, magnetism*)

$C_4H_{17}B_{10}^{\oplus}$ – $C_4H_{17}N_5O_2Ru^{2\oplus}$

IC-004400

$C_4H_{17}B_{10}^{\oplus}$

7,9-Dimethyl-7,9-dicarbadodecaborate(1−)



R = CH_3

M 173.2 (ion)
nido-. Two isomers known- 'stable' and 'unstable', latter (shown) reacts with many metal complexes.
$MePh_3P$ salt: Colourless cryst. (1,2-dibromoethane/Et_2O).
Sol. 1,2-dibromoethane.

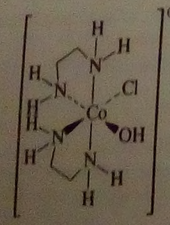
Dunks, G.B. *et al, J. Chem. Soc., Chem. Commun.*, 1972, 899 (*synth*)
Dunks, G.B. *et al, J. Am. Chem. Soc.*, 1973, **95**, 3174 (*synth*)
Getman, T.D. *et al, Inorg. Chem.*, 1990, **29**, 158 (*cryst struct*)

$C_4H_{17}ClCoN_4O^{\oplus}$

IC-004401

Chlorobis(ethylenediamine)hydroxycobalt(*III*)(1+)

*Chlorobis(1,2-ethanediamine-*N,N′*)hydroxycobalt(1+), 9CI*



cis-form

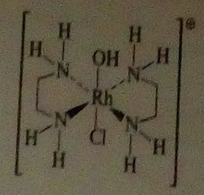
M 231.5 (ion)
cis-form [54453-02-0]
Bromide: Brown-violet cryst. (EtOH aq./Et_2O).
trans-form [20142-32-9]
Chloride: [20941-80-4].
Grey cryst. (EtOH aq.).
[19428-61-6]

Baldwin, M.E. *et al, J. Chem. Soc.*, 1960, 4369; 1961, 4637 (*synth, ir*)
Chan, S.C. *et al, J. Chem. Soc.*, 1962, 4531 (*synth*)
Dittmar, E.A. *et al, J. Am. Chem. Soc.*, 1968, **90**, 1468 (*hydrol*)

$C_4H_{17}ClN_4ORh^{\oplus}$

IC-004402

Chlorobis(ethylenediamine)hydroxyrhodium(*III*)(1+)



M 275.5 (ion)
trans-Octahedral.
Tetraphenylborate: No phys. props. reported.

Gillard, R.D., *J. Chem. Soc. A*, 1970, 3126 (*synth, ir*)

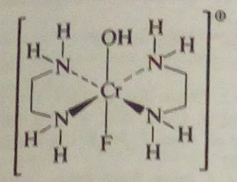
$C_4H_{17}CrFN_4O^{\oplus}$

IC-004403

Bis(ethylenediamine)fluorohydroxychromium(*III*)(1+)

*Bis(1,2-ethanediamine-*N,N′*)fluorohydroxychromium*(III)*(1+), 1ICl*

[85826-81-9]



M 208.1 (ion)
trans-Octahedral cation.
*Diaquabis(1,2-ethanediamine-*N,N′*)chromium(3+) perchlorate (2:1:5):* [85826-83-1].
Cryst. + $2H_2O$. Struct. consists of complex cations linked by strong hydrogen bonds in infinite chains.

[91739-94-5]

Solans, X. *et al, Cryst. Struct. Commun.*, 1982, **11**, 1199 (*cryst struct*)

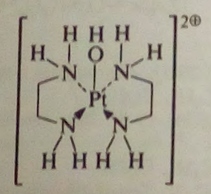
$C_4H_{17}N_4OPt^{2\oplus}$

IC-004404

Bis(ethylenediamine)hydroxyplatinum(2+)

Bis(ethanediamine)hydroxyplatinum(III)*(2+), 10Cl*

[74592-11-3]



M 332.2 (ion)
Example of unusual Pt(*III*) sp. Synth. from $[Pt(en)_2]^{2\oplus}$ + OH radical. Formed in soln. but not isol.

Waltz, W.L. *et al, Inorg. Chem.*, 1980, **19**, 3284.

$C_4H_{17}N_5O_2Ru^{2\oplus}$

IC-004405

Bis(ethylenediamine)(hydroxy)(nitrosyl)ruthenium(2+)

*Bis(1,2-ethanediamine-*N,N′*)hydroxy(nitrosyl)ruthenium(2+)*

$[Ru(NO)(OH)(NH_2CH_2CH_2NH_2)_2]^{2\oplus}$

M 268.2 (ion)
Salts of $Cl^{\ominus}$, $Br^{\ominus}$, $I^{\ominus}$, $NO_3^{\ominus}$, $ClO_4^{\ominus}$ and $SO_4^{2\ominus}$ reported in the early literature; struct. unknown.

Werner, A. *et al, Helv. Chim. Acta*, 1920, **3**, 737 (*synth*)
Charonnat, R., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1924, **178**, 1279, 1423 (*synth*)
Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 225 (*synth*)

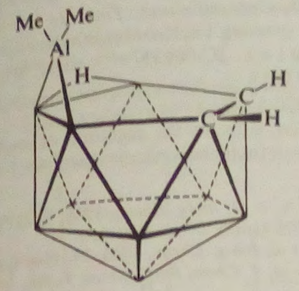
$C_4H_{18}AlB_9$

IC-004406

[Dodecahydro-7,8-dicarbaundecaborato(1−)-*H*^{9},*H*^{10}] dimethylaluminium

*3,4-μ-Dimethylaluminio-1,2-dicarba-*nido*-undecaborane(13)*

[11098-56-9]



M 190.4
Fluxional H bridge proposed. Colourless cryst. (C_6H_6). Mp 120-122°. Subl. *in vacuo*.

▷ Explodes with water.

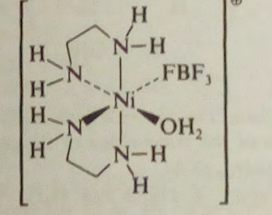
Young, D.A.T. *et al, J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, pmr, nmr*)
Churchill, M.R. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1314 (*struct*)

$C_4H_{18}BF_4N_4NiO^{\oplus}$

IC-004407

Aquabis(1,2-ethanediamine-*N,N′*)(tetrafluoroborato-*F*) nickel(*II*)(1+), 9CI

Tetrafluoroborato(aqua)bis(ethylenediamine)nickel(II)



M 283.7 (ion)
cis-Octahedral at Ni.
Tetrafluoroborate: [37651-45-9].
Blue orthorhombic prisms.

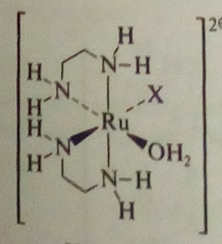
Tomlinson, A.A.G. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1671 (*synth, cryst struct, ir, uv*)

$C_4H_{18}BrN_4ORu^{2\oplus}$

IC-004408

Aquabromobis(ethylenediamine)ruthenium(*III*)(2+)

*Aquabromo(1,2-ethanediamine-*N,N′*)ruthenium(2+), 9CI.*
Aquabromobis(1,2-diaminoethane)ruthenium(III)*(2+)*



cis-form

X = Br

M 319.1 (ion)
Both *cis* and *trans* isomers have been generated in soln., but only the *cis* form has been isol. Sol. H_2O. Both forms undergo ready hydration and anation.

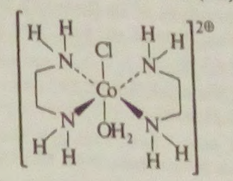
cis-form [31274-34-7]
Bis(4-methylbenzenesulfonate): Tosylate
Prepd. by treating Dibromobis(ethylenediamine) ruthenium(*III*)(1+), IC-004332 with silver tosylate. Brown cryst. + $1H_2O$.
trans-form [73285-23-1]
Prepd. in aq. soln. by the aquation of *trans*-form of Dibromobis(ethylenediamine)ruthenium(*III*)(1+), IC-004332.

Broomhead, J.A. *et al, Inorg. Chem.*, 1968, **7**, 2519; 1971, **10**, 85; 1975, **14**, 2575 (*synth, ir, uv, aquation*)
Poon, C.-K. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 128 (*electrochem*)

$C_4H_{18}ClCoN_4O^{2\oplus}$

IC-004409

Aquachlorobis(ethylenediamine)cobalt(*III*)(2+)



M 232.5 (ion)
trans-form
Dithionate: [83835-69-2].
Formed from $[Co(en)_2(CO_3)]Cl$ and conc. HCl. Grey-green fluffy needles + $1H_2O$.

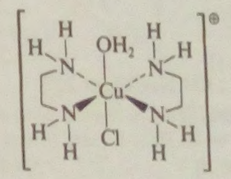
Inorg. Synth., 1982, **21**, 125 (*synth, uv*)

$C_4H_{18}ClCuN_4O^{\oplus}$

IC-004410

Aquachlorobis(ethylenediamine)copper(*II*)(1+)

*Aquachlorobis(1,2-ethanediamine-*N,N′*)copper*(II)*(1+), 11Cl, 10Cl, 9Cl*



M 237.2 (ion)
trans-Octahedral.
Chloride: [21255-25-4].
Deliquescent, purple needles (EtOH). Mp 218°. Forms a monohydrate.

[53224-04-7]

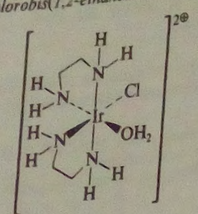
Chattaway, F.W. *et al, J. Chem. Soc.*, 1937, 947 (*synth*)
Jonassen, H.B. *et al, J. Am. Chem. Soc.*, 1949, **71**, 1553 (*synth, uv*)
Ball, R.D. *et al, J. Chem. Soc. A*, 1967, 1435 (*cryst struct*)
Misra, B.N. *et al, Z. Naturforsch., A*, 1973, **28**, 246 (*esr*)
Miskowski, V.M. *et al, J. Am. Chem. Soc.*, 1976, **98**, 8344 (*uv*)
Gabelica, Z., *Spectrochim. Acta, Part A*, 1976, **32**, 337 (*ir*)

IC-004411

$C_4H_{18}ClIrN_4O^{2\oplus}$

Aquachlorobis(ethylenediamine)iridium(*III*)(2+)

Aquachlorobis(1,2-ethanediamine-N,N′)iridium(2+), 9CI



cis-form

M 365.8 (ion)

Octahedral geometry.

cis-form [74034-28-9]

Prepd. by photolysis of *cis*-$[Ir(en)_2Cl_2]^{\oplus}$ in aq. soln. Present in ionic form in aq. soln. Not isol.

trans-form [45838-63-9]

Perchlorate: White cryst. Sol. H_2O.

▷ Potentially explosive.

Bauer, R.A. *et al, Inorg. Chem.*, 1969, **8**, 2231 (*synth, uv*)

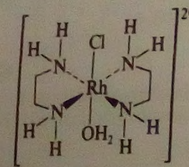
Sarvari, M.T. *et al, Inorg. Chem.*, 1980, **19**, 2640 (*synth, uv, photochem*)

IC-004412

$C_4H_{18}ClN_4ORh^{2\oplus}$

Aquachlorobis(ethylenediamine)rhodium(*III*)(2+)

Aquachlorobis(1,2-ethanediamine-N,N′)rhodium(2+), 9CI



trans-form

M 276.5 (ion)

cis-form [53368-47-1]

pK_a 7.65 (aq. 1.0*M* $NaClO_4$ at 25°).

Dithionate: [107890-72-2].

Yellow cryst. + $1H_2O$.

trans-form [15337-41-4]

pK_a 6.48 (aq. 1.0*M* $NaClO_4$ at 25°).

Diperchlorate: [55683-58-4].

Pale yellow cryst. Sol. Me_2CO, H_2O.

Dithionate: [107890-71-1].

Orange-yellow cryst. + $1H_2O$.

Burgess, C. *et al, Inorg. Chim. Acta*, 1975, **13**, 35 (*synth, ir, uv, raman*)

Jakse, F.P., *Inorg. Chim. Acta*, 1978, **27**, 225 (*cmr*)

Skibsted, L.H. *et al, Inorg. Chem.*, 1987, **26**, 1708 (*dithionates, uv-vis, photochem*)

IC-004413

$C_4H_{18}ClN_4ORu^{2\oplus}$

Aquachlorobis(ethylenediamine)ruthenium(*III*)(2+)

Aquachlorobis(1,2-ethanediamine-N,N′)ruthenium(2+), 9CI.

Aquachlorobis(1,2-diaminoethane)ruthenium(III)(*2+*)

As Aquabromobis(ethylenediamine)ruthenium(*III*)(2+), IC-004408 with

X = Cl

M 274.7 (ion)

Both *cis* and *trans* - isomers have been generated in soln., but only the *cis*-form has been isol. Sol. H_2O. Both forms undergo ready hydration, anation and a photo-induced isomerisation.

cis-form [31274-35-8]

Ru—N 210, Ru—Cl 232.3, Ru—O 209.3 pm.

Bis(4-methylbenzenesulfonate): Tosylate

Prepd. by treating Dichlorobis(ethylenediamine) ruthenium(1+), IC-004357with silver tosylate. Yellow cryst. + $1H_2O$.

trans-form [55870-37-6]

Prepd. in aq. soln. by the aquation of *trans*-form of Dichlorobis(ethylenediamine)ruthenium(1+), IC-004357.

Broomhead, J.A. *et al, Inorg. Chem.*, 1968, **7**, 2519; 1971, **10**, 85; 1975, **14**, 2575 (*synth, ir, uv, aquation*)

Rerek, M.E. *et al, Inorg. Chem.*, 1980, **19**, 2646 (*photol*)

Poon, C.-K. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 128 (*electrochem*)

Ceulemans, A. *et al, Inorg. Chem.*, 1983, **22**, 1113 (*synth*)

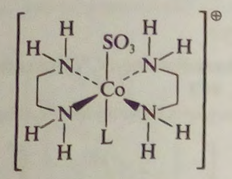
Hambley, T.W. *et al, Aust. J. Chem.*, 1984, **37**, 435 (*cryst struct, hydration, hydrol*)

IC-004414

$C_4H_{18}CoN_4O_4S^{\oplus}$

Aquabis(ethylenediamine)[sulfito(2−)-*S*]cobalt(*III*)(1+)

[28530-11-2]



L = OH_2

M 277.2 (ion)

Octahedral cation. The Co—OH_2 distance is long (203.7 pm) because of the *trans*-effect of the sulfite ligand.

Perchlorate: [24492-59-9].

Red-brown cryst. + $1H_2O$. Sol. H_2O.

▷ Potentially explosive.

Baldwin, M.E. *et al, J. Chem. Soc.*, 1961, 3123 (*synth*)

Stranks, D.R. *et al, Inorg. Chem.*, 1970, **9**, 751 (*kinetics*)

Maslen, E.N. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 327 (*cryst struct*)

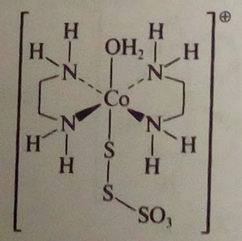
IC-004415

$C_4H_{18}CoN_4O_4S_3^{\oplus}$

Aqua[(dithioperoxy)monosulfato(2−)]bis(1,2-ethanediamine-*N*,*N*′)cobalt(1+), 10CI

Aqua(disulfane monosulfonato)bis(ethylenediamine) cobalt(III)(*1+*)

[75936-25-3]



M 341.3 (ion)

Prob. ion formed on soln. of Chlorobis(ethylenediamine) sulfitocobalt(*III*), IC-004335. Mod. stable complex containing the v. reactive disulfane mono-sulfonate ligand. Cation gives yellow-brown colour in aq. soln. Not isol.

Mittleman, J.P. *et al, J. Chem. Soc., Chem. Commun.*, 1980, 733 (*synth, props*)

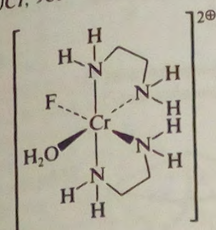
IC-004416

$C_4H_{18}CrFN_4O^{2\oplus}$

Aquabis(ethylenediamine)fluorochromium(*III*)(2+), 8CI

Aquabis(1,2-ethanediamine-N,N′)fluorochromium(III)

Aquabis(1,2-ethanediamine-N,N′)fluorochromium(2+),10CI, 9CI



Δ,*cis-form*

M 209.2 (ion)

Octahedral complex.

Δ-cis-form

Bis-tetraphenylborate: [69880-71-3].

$[\alpha]_D$ 0°, $[\alpha]_{546}$ −186°, $[\alpha]_{520}$ −162° (c, 0.3 in Me_2CO).

(±),*cis-form* [34431-44-2]

Diiodide: [59765-91-2].

Orange solid + $1H_2O$.

Bis-tetraphenylborate: [69847-10-5].

Pink solid + 1.5 H_2O.

trans-form [28101-89-5]

Dichloride: [19581-07-8].

Fluffy pink solid + H_2O. Sol. H_2O.

Dibromide: [15697-74-2].

Pink solid + H_2O.

Diiodide: [19581-06-7].

Orange cryst. + 0.5H_2O. Sol. H_2O. Dehydrates at 160-170° on heating for 12 hr. to form purple cryst. $[Cr(en)_2FI]I$.

Dithiocyanate: [19581-08-9].

Orange powder. Sol. H_2O.

Diperchlorate: [15688-01-4].

Bright orange cryst. + H_2O. Sol. H_2O. Ir ν_{CrN}475, 445; ν_{CrF} 365 cm^{-1}.

▷ Potentially explosive.

[26318-83-2, 62792-39-6]

Vaughn, J.W. *et al, Inorg. Chem.*, 1968, **7**, 736; 1976, **15**, 2320; 1979, **18**, 1509 (*synth, resoln*)

Brown, D.H. *et al, Inorg. Nucl. Chem. Lett.*, 1969, **5**, 991 (*ir*)

Vaughn, J.W. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1977, **7**, 165 (*synth, cis-form*)

IC-004417

$C_4H_{18}CrN_4O_4$

Bis(acetato-*O*)tetraamminechromium(*II*), 10CI

Chromium(II) *acetate tetraammine*

[75576-29-3]

$Cr(OAc)_2(NH_3)_4$

M 238.2

Octahedral at Cr. Obt. by action of liq. ammonia on Chromium(*II*) acetate, IC-004009. Violet, air-sensitive solid. Loses ammonia to give Chromium(*II*) acetate, IC-004009. μ_{eff} = 4.73μ_B (295K).

Larkworthy, L.F. *et al, Inorg. Nucl. Chem. Lett.*, 1980, **16**, 427 (*synth*)

IC-004418

$C_4H_{18}IN_4ORu^{2\oplus}$

Aquabis(ethylenediamine)iodoruthenium(*III*)(2+)

Aquabis(1,2-ethanediamine-N,N′)iodoruthenium(2+), 9CI.

Aquabis(1,2-diaminoethane)iodoruthenium(III)(*2+*)

As Aquabromobis(ethylenediamine)ruthenium(*III*)(2+), IC-004408 with

X = I

M 366.1 (ion)

cis-form [87655-45-6]

Bis(4-methylbenzenesulfonate): Tosylate

Synth. by treating Bis(ethylenediamine) diiodoruthenium(*III*)(1+), IC-004374 with silver tosylate. Purple cryst. Sol. H_2O.

trans-form [87725-97-1]

Prepd. in aq. soln. by the aquation of the *trans*-form of Bis(ethylenediamine)diiodoruthenium(*III*)(1+), IC-004374. Sol. H_2O.

Broomhead, J.A. *et al, Inorg. Chem.*, 1968, **7**, 2519 (*synth, uv, aquation*)

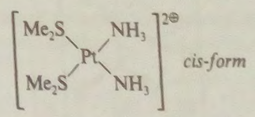
Poon, C.K. *et al, Inorg. Chem.*, 1983, **22**, 3893 (*synth, uv, photohem*)

IC-004419

$C_4H_{18}N_2PtS_2^{2\oplus}$

Diamminebis(dimethyl sulfide)platinum(*II*)

Diamminebis[thiobis(methane)]platinum(II)(*2+*), *10CI*



cis-form

M 353.4 (ion)

Kinetic studies show substitutions give loss of first NH_3, than either loss of second NH_3 or an SMe_2.

cis-form [90670-30-7]

Chloride: [62800-71-9].

Props. not described.

trans-form [90760-61-5]

Annibale, G. *et al, Inorg. Chim.*, 1984, **23**, 2705, 2829 (*synth*)

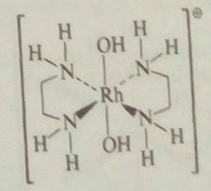
IC-004420

$C_4H_{18}N_4O_2Rh^{\oplus}$

Bis(ethylenediamine)dihydroxyrhodium(*III*)(1+)

Bis(1,2-ethanediamine-N,N′)dihydroxyrhodium(III)(*1+*), *9CI*

[55683-53-9]



M 257.1 (ion)

trans-Octahedral cation.

Perchlorate: Sol. H_2O.

▷ Potentially explosive.

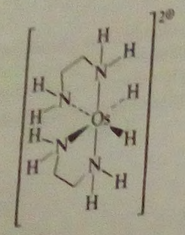
Gillard, R.D. *et al*, *J. Chem. Soc. A*, 1970, 3126 (*synth, electrochem, reactions*)
Burgess, C. *et al*, *Inorg. Chim. Acta*, 1975, **13**, 35 (*synth, uv*)

IC-004421

$C_4H_{18}N_4Os^{2\oplus}$

Bis(ethylenediamine)dihydroosmium(*IV*)(2+)

[57345-94-5]



M 312.4 (ion)
cis-Octahedral.
Tetrachlorozincate(2−): [34410-57-6].
Synth. by reduction of $[Os(en)_2O_2]Cl_2$ with Zn in HCl.
Bright yellow solid. Ir ν_{Os-H} 2150 cm^{-1}.

[45838-80-0]

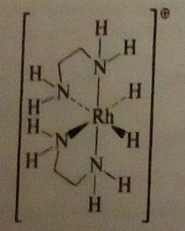
Malin, J.M. *et al*, *Inorg. Chem.*, 1971, **10**, 2403 (*synth, ir, pmr, uv*)
Suvana, S.S.L. *et al*, *Spectrosc. Lett.*, 1973, **6**, 323.
Coelho, A.L., *Inorg. Chim. Acta*, 1975, **14**, L41 (*synth*)
Malin, J.M., *Inorg. Chim. Acta*, 1980, **45**, L87 (*synth, use*)

IC-004422

$C_4H_{18}N_4Rh^{\oplus}$

Bis(ethylenediamine)dihydridorhodium(*III*)(1+)

*Bis(1,2-ethanediamine-*N,N′*)dihydrorhodium(1+)*



M 225.1 (ion)
cis-Octahedral.
Tetraphenylborate: Pale brown solid. Sol. H_2O.

Gillard, R.D. *et al*, *J. Chem. Soc.*, 1963, 3594 (*synth, uv, ir*)
Osborn, J.A. *et al*, *J. Chem. Soc.*, 1964, 3168 (*pmr*)

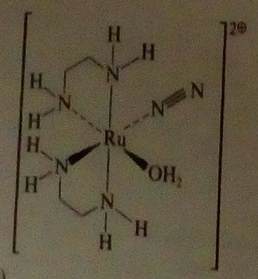
IC-004423

$C_4H_{18}N_5ORu^{2\oplus}$

Aqua(dinitrogen)(ethylenediamine)ruthenium(*II*)(2+)

*Aqua(dinitrogen)bis(1,2-ethanediamine-*N,N′*)ruthenium(2+), 9CI*; *Aquabis(1,2-diaminoethane)(dinitrogen)ruthenium*(II)

[53177-07-4]



M 267.2 (ion)

cis-Octahedral. Prepd. by treating *cis*-Azido(dinitrogen) bis(ethylenediamine)ruthenium(*II*)(1+), IC-004397 with nitrous acid, by treating Tris(ethylenediamine) ruthenium(3+), IC-005519 with NO in basic aq. soln., or by treating *cis*-$[Ru(en)_2(OH_2)_2]^{2\oplus}$ with N_2. Sol. H_2O. Ir ν_{N_2} 2130 cm^{-1}.
Bis-tetraphenylborate: Solid.

[35668-30-5]

Kane-Maguire, L.A.P. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5295; 1970, **92**, 5865 (*synth, ir, uv*)
Kane-Maguire, L.A.P., *J. Inorg. Nucl. Chem.*, 1971, **33**, 3964 (*synth, kinetics*)
Pell, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1974, 259 (*synth, ir*)

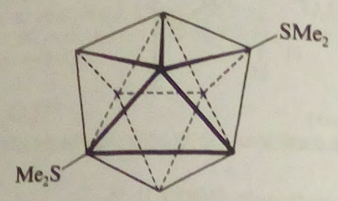
IC-004424

$C_4H_{19}B_9S_2$

5,7-Bis(dimethyl sulfide)nonaborane(7)

5,7-Bis[thiobis[methane]]nonaborane(7)

[81343-16-0]



M 228.6
closo-. Colourless cryst. (C_6H_6/hexane). Sol. $CHCl_3$, C_6H_6.

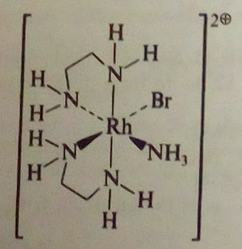
Bray, D.D. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 957 (*cryst struct*)
Wong, E.H. *et al*, *Inorg. Chem.*, 1982, **21**, 4022 (*synth, struct, B-11 nmr, pmr, props, ir*)

IC-004425

$C_4H_{19}BrN_5Rh^{2\oplus}$

Amminebromobis(ethylenediamine)rhodium(*III*)(2+)

[62153-07-5]



cis-form

M 320.0 (ion)

cis-form

Bis-nitrate: Appearance not described. Sol. H_2O, dioxan.

trans-form

Bis-nitrate: Appearance not described. Sol. H_2O, dioxan.

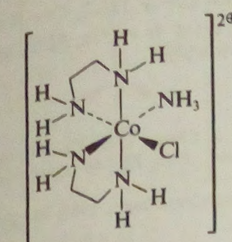
Clark, S.F. *et al*, *Inorg. Chem.*, 1979, **18**, 3394 (*synth, uv, cmr, photochem*)

IC-004426

$C_4H_{19}ClCoN_5^{2\oplus}$

Amminechlorobis(ethylenediamine)cobalt(*III*)(2+)

*Amminechlorobis(1,2-ethanediamine-*N,N′*)cobalt*(III)(*2+*), *10Cl*



cis-form

M 231.6 (ion)

cis-form [15392-82-2]
Has been resolved.
Dichloride: [14408-61-8].
Red prisms. Sl. sol. H_2O.
Dinitrate: Red cryst. Sl. sol. H_2O.
Diperchlorate: [15280-85-0].
Red cryst. Potentially expolsive.
d-3-Bromocamphor-9-sulfonate: [69256-84-4].
Deep red cryst. + H_2O. Abs. config. detd. for cation, Co—NH_3 200, Co—Cl 227, Co—NH_2 196-200 pm; (+)-form has Δ configuration.

trans-form [19314-39-7]
Dichloride: [38833-25-9].
Blue-red cryst. + $1\frac{1}{2}H_2O$. Sl. sol. H_2O.
Diperchlorate: [71380-87-5].
Red cryst. (EtOH aq.).

[18660-69-0, 58437-87-9, 58560-82-0]

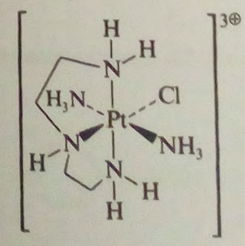
Jorgensen, S.M., *J. Prakt. Chem.*, 1890, **41**, 458 (*synth, cis-form*)
Werner, A., *Ber.*, 1911, **42**, 1890 (*synth, cis-form, resoln*)
Werner, A. *et al*, *Justus Liebigs Ann. Chem.*, 1912, **386**, 55, 165, 170, 228 (*cis-form, synth*)
Kuroya, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1940, **15**, 427 (*uv-vis*)
Basolo, F. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 819 (*reactions, uv-vis*)
Nyholm, R.S. *et al*, *J. Chem. Soc.*, 1956, 1707 (*synth, reactions*)
Brushmiller, J.G. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 111 (*uv-vis*)
Gmelin Handbook Inorg. Chem., Syst. No. 58, 1964, **B2**, 468 (*rev, bibl*)
Kuramoto, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1978, **51**, 3196 (*cryst struct*)
Miyshi, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 3845 (*cis-form, abs config*)
Balt, S. *et al*, *Inorg. Chem.*, 1985, **24**, 3347 (*substn*)
Balt, S. *et al*, *Transition Met. Chem.*, 1985, **10**, 164 (*pmr*)

IC-004427

$C_4H_{19}ClN_5Pt^{3\oplus}$

Diamminechloro(diethylenetriamine)platinum(*IV*)(3+)

[N-(*2-Aminoethyl*)-*1,2-ethanediamine*]*diamminechloroplatinum*(3+), *9CI*



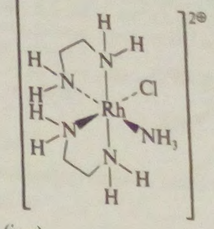
M 367.7 (ion)
Believed to have *mer*-configuration; NH_3 groups presumed *trans*.
Trichloride: [56110-92-0].

$C_4H_{19}Cl_4N_5Pt$ M 474.1
V. hygroscopic pale yellow solid.
Mochida, I. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 3021.

IC-004428

$C_4H_{19}ClN_5Rh^{2\oplus}$

Ammine(chloro)bis(ethylenediamine)rhodium(*III*)(2+)



cis-form

M 275.5 (ion)
Octahedral.

cis-form [67047-31-8]
Chloride: [65794-88-9].
Pale yellow solid. Sol. H_2O.
Nitrate: [70178-70-0].
Pale yellow solid. Sol. dioxan.

trans-form [61697-84-5]
Chloride: Pale yellow solid.
Nitrate: [65802-28-0].
Pale yellow solid. Sol. dioxan.

[65794-89-0, 65794-90-3]

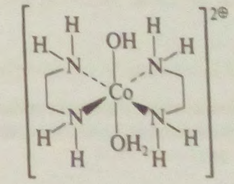
Johnson, S.A. *et al*, *Inorg. Chem.*, 1962, **1**, 925 (*synth, ir, uv*)
Ogino, H. *et al*, *Inorg. Chem.*, 1978, **17**, 1118 (*synth, uv, pmr*)
Jakse, F.P. *et al*, *Inorg. Chim. Acta*, 1978, **27**, 225 (*uv, cmr*)

IC-004429

$C_4H_{19}CoN_4O_2^{2\oplus}$

Aquabis(ethylenediamine)hydroxycobalt(*III*)(2+), 8Cl

*Aquabis(1,2-ethanediamine-*N,N′*)hydroxycobalt*(III)(*2+*)



M 214.1 (ion)

trans-form

Dinitrate: [16570-48-2].
Not isolated, used for mechanistic study.

Chan, S. *et al*, *Inorg. Chem.*, 1971, **10**, 1317 (*synth, kinetics*)

IC-004430

$C_4H_{19}CoN_5O_3S^{\oplus}$

Amminebis(ethylenediamine)sulfitocobalt(*III*)(1+)

*Amminebis(1,2-ethanediamine-*N,N′*)[sulfito(2−)-*S*]cobalt(1+), 10Cl*

As Aquabis(ethylenediamine)[sulfito(2−)-*S*]cobalt(*III*) (1+), IC-004414 with

L = NH_3

M 276.2 (ion)
Octahedral at Co.
Chloride: Yellow-brown needles. Sol. H_2O.
Perchlorate: [74876-01-0].
Cryst.

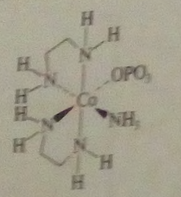
▷ Potentially explosive.

Baldwin, M.E., *J. Chem. Soc.*, 1961, 3123 (*synth, ir, uv*)
Raston, C.L. *et al, Aust. J. Chem.*, 1980, **33**, 1123 (*cryst struct*)

IC-004431

$C_4H_{19}CoN_5O_4P$

Amminebis(ethylenediamine)phosphatocobalt(*III*), 8Cl



cis-form

M 291.1
Octahedral.

cis-form [33031-22-0]
Pink solid + $3H_2O$. Sol. F_3CCOOH.

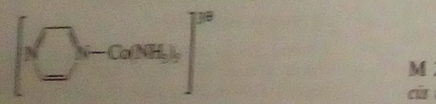
trans-form [33031-23-1]
Deep red cryst. + $5H_2O$. Sol. F_3CCOOH.

Linssin, S.F. *et al, Inorg. Chem.*, 1971, **10**, 1254 (*synth, pmr, uv, kinetics*)

IC-004432

$C_4H_{19}CoN_7^{3\oplus}$

Pentaammine(pyrazine-*N*)cobalt(*III*)(3+), 10Cl



M 224.1 (ion)
Trigenhlorate: [70128-40-2].
Yellow-orange needles. Sol. H_2O.
▷ Potentially explosive.

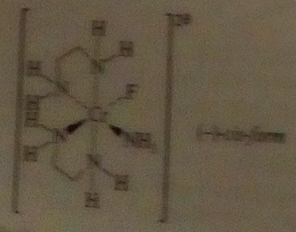
Malin, J.M. *et al, J. Am. Chem. Soc.*, 1970, **100**, 2097 (*synth, kinetics, pmr, uv*)

IC-004433

$C_4H_{19}CrFN_7^{3\oplus}$

Amminebis(ethylenediamine)fluorochromium(*III*)(2+)

Amminebis(1,2-ethanediamine-N,N')fluorochromium(III)
(2+), 1ICl, 1HCl, 9Cl
[58410-71-2]



(−)-*cis-form*

M 208.2 (ion)
Pseudo-octahedral geometry.
(−)-*cis-form*
Δ-*form*
Diperchlorate: [84367-53-3].
Orange solid. $[\alpha]_{546}$ −53.4°, $[\alpha]_{436}$ −106.8° (0.25% aq. soln. at r.t.).
(±)-*cis-form*
Diperchlorate: [58437-81-3].
Orange solid. Ir *v* 540s, 519m cm^{-1}.
Dibromide: [84279-86-7].
Orange solid.
Chloride, iodide: [84279-84-5].
Solid.

trans-form
Interatomic distances: Cr—F 186.2, Cr—N 209.3 pm.
Diperchlorate: Orange cryst. Ir *v* 551s, 522m cm^{-1}.
Chloride, iodide: [84279-85-6].
Solid.

[58437-80-2]

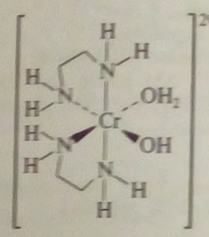
Wong, C.F.C. *et al, Can. J. Chem.*, 1975, **53**, 3388 (*synth*)
Vaughn, J.W., *Inorg. Chem.*, 1983, **22**, 844 (*synth, resoln, cis-form, hplc, uv-vis*)
Beveridge, K.A. *et al, Acta Crystallogr.*, 1985, **41**, 899 (*cryst struct, trans-form*)

IC-004434

$C_4H_{19}CrN_4O_2^{2\oplus}$

Aquabis(ethylenediamine)hydroxychromium(*III*)(2+), 8Cl

Aquabis(1,2-ethanediamine-N,N')hydroxychromium(III)
(2+), 1ICl, 1OCl, 9Cl



cis-form

M 207.2 (ion)
cis and *trans* isomers known. Formed on photoaquation of $[Cr(en)_3]^{3\oplus}$.

cis-form
Dithionate: [34076-61-4].
V. stable red cryst. + H_2O. Insol. H_2O. In strong acid or base, gives *cis*-diaqua and *cis*-dihydroxo species respectively.
Bis-tetraphenylborate: [66350-08-1].
Obt. on irradiation of solid $[Cr(en)_3](BPh_4)_3.2H_2O$. Pink solid.

trans-form [31253-65-3]
Dibromide: [15654-70-3].
Synth. from mixing *trans*-$[Cr(en)_2(OH_2)_2]Br_3$, NaBr and Py. Orange cryst. + H_2O.

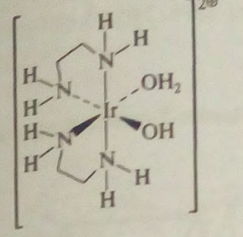
[52524-45-5, 62728-44-3]

Woldbye, F., *Acta Chem. Scand.*, 1958, **12**, 1079 (*ion, equilibria*)
Hughes, M.N. *et al, J. Chem. Soc. A*, 1967, 592 (*ir*)
Kiens, R.L. *et al, Inorg. Chim. Acta*, 1973, **7**, 685 (*trans-bromide salt, synth, uv-vis*)
Jackson, W.G. *et al, Inorg. Chim. Acta*, 1977, **22**, 111 (*kinetics*)
Inorg. Synth., 1978, **18**, 75 (*synth*)
Gillard, R.D. *et al, Transition Met. Chem.*, 1978, **3**, 44 (*BPh_4 salt*)

IC-004435

$C_4H_{19}IrN_4O_2^{2\oplus}$

Aquabis(ethylenediamine)hydroxyiridium(*III*)(2+)



cis-form

M 347.4 (ion)
Octahedral geometry at Ir.

cis-form
Prepd. by base hydrol. of *cis*-$[Ir(en)_2Cl_2]Cl$.
Dithionate: [91947-50-1].
White cryst.
Diperchlorate: Cream solid. Sol. H_2O.
▷ Potentially explosive.

trans-form
Prepd. by base hydrol. of *trans*-$[Ir(en)_2Cl_2]Cl$.
Diperchlorate: [92609-56-8].
Cream coloured solid. Sol. H_2O.
▷ Potentially explosive.

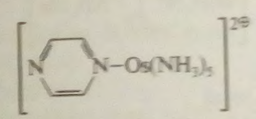
Galsboel, F. *et al, Acta Chem. Scand., Ser. A*, 1984, **38**, 141 (*synth, uv, electrochem*)

IC-004436

$C_4H_{19}N_7Os^{2\oplus}$

Pentaamminepyrazineosmium(*II*)(2+)

[70252-44-7]



M 355.4 (ion)
Obt. by reduction of the Os(*III*) species.
Dichloride: [115244-81-0].
Synth. from $[Os(NH_3)_5(OSO_2CF_3)](CF_3SO_3)_2$ and excess pyrazine in triethyl phosphite. Dark brown solid.
Diiodide: [115244-82-1].
Synth. from $[Os(NH_3)_5(pz)](CF_3SO_3)_3$ and Zn(Hg) in Me_2CO, followed by addition of $[Bu_4N]I$.

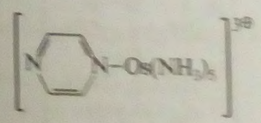
Sen, J. *et al, Acta Chem. Scand., Ser. A*, 1979, **33**, 125 (*synth, electrochem*)
Johnson, C.R. *et al, Inorg. Chem.*, 1983, **22**, 1117 (*uv*)
Farquharson, S. *et al, Spectrochim. Acta, Part A*, 1984, **40**, 907.
Weaver, M.J. *et al, J. Chem. Phys.*, 1985, **82**, 4867 (*synth, raman*)
Creutz, C. *et al, Inorg. Chem.*, 1987, **26**, 2995 (*uv, electrochem*)
Lay, P.A. *et al, Inorg. Chem.*, 1988, **27**, 2848 (*synth, electrochem, uv*)

IC-004437

$C_4H_{19}N_7Os^{3\oplus}$

Pentaamminepyrazineosmium(*III*)(3+)

[83781-34-4]



M 355.4 (ion)
Trichloride: [70252-37-8].
Synth. by reaction of $[OsN_2(NH_3)_4]Cl_2$ with silver tosylate in triethylphosphate, followed by addition of pyrazine.
Tris(trifluoromethanesulfonate): [83781-35-5].
[83781-40-2]

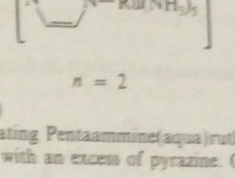
Sen, J. *et al, Acta Chem. Scand., Ser. A*, 1979, **33**, 125 (*synth, uv, pKa*)
Lay, P.A. *et al, J. Am. Chem. Soc.*, 1982, **104**, 7658 (*synth, uv*)
Farquharson, S. *et al, J. Am. Chem. Soc.*, 1984, **106**, 5123 (*raman*)
Farquharson, S. *et al, Spectrochim. Acta, Part A*, 1984, **40**, 907 (*kinetics, raman*)
Lay, P.A. *et al, Inorg. Chem.*, 1988, **27**, 2848 (*synth, electrochem, uv*)

IC-004438

$C_4H_{19}N_7Ru^{2\oplus}$

Pentaammine(pyrazine-*N*^{4})ruthenium(*II*)(2+), 10Cl

[19471-65-9]



$n = 2$

M 266.3 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with an excess of pyrazine. Orange-red aq. soln.

Diiodide: [41481-92-9].
$C_4H_{19}I_2N_7Ru$ M 520.1
Diperchlorate: [41481-90-7].
Orange-red cryst. (H_2O).
Bis-tetrafluoroborate: [41481-91-8].
[76584-37-7]

Ford, P.C. *et al, J. Am. Chem. Soc.*, 1968, **90**, 1187 (*synth, uv, electrochem*)
Creutz, C. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1086 (*synth, uv, electrochem, ir*)

IC-004439

$C_4H_{19}N_7Ru^{3\oplus}$

Pentaammine(pyrazine-*N*^{4})ruthenium(*III*)(3+), 10Cl

[38139-16-1]

As Pentaammine(pyrazine-*N*^{4})ruthenium(*II*)(2+), IC-004438 with

$n = 3$

M 266.3 (ion)
Prepd. by oxidising Pentaammine(pyrazine-*N*^{4})ruthenium(*II*)(2+), IC-004438 with PbO_2/H_2SO_4.
Yellow aq. soln.

Tribromide: [70589-27-8].
Yellow cryst. + HBr.
Tris-(4-methylbenzenesulfonate): [41557-34-0].
Light yellow cryst. + $3H_2O$.

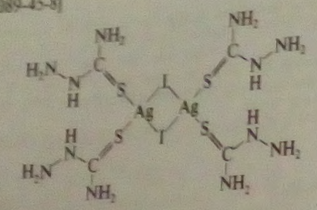
Creutz, C. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1086 (*synth, uv, vis, electrochem*)

IC-004440

$C_4H_{20}Ag_2I_2N_{12}S_4$

Tetrakis(hydrazinecarbothioamide-*S*)di-μ-iododisilver(*I*), 12CI

[108089-45-8]



M 834.0

Cryst.

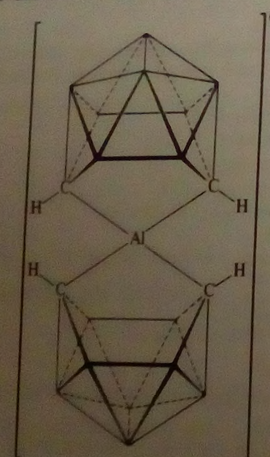
Nardelli, M. *et al, Ric. Sci.*, 1965, **35**, 480 (*synth*)

Bonamartini, A.C. *et al, Acta Crystallogr., Sect. C*, 1987, **43**, 407 (*struct*)

IC-004441

$C_4H_{20}AlB_{16}^{\ominus}$

Bis(6,9-dicarbadecaborane(12)-6,9-diyl)aluminate(1−)



M 268.1 (ion)

Na salt: [106006-55-7].

Pale-yellow microcryst. Mod. stable in dry air. Mp >300°. Ir ν_{B-H} 2543 cm^{-1}.

Bis(triphenylphosphine)iminium salt: [106006-57-9].

White cryst., stable in dry air. Reacts slowly with water, faster with wet Me_2CO. Sol. CH_2Cl_2. Mp >300°.

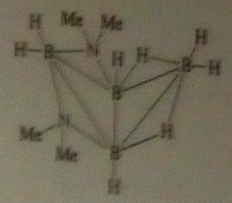
Schubert, D.M. *et al, Organometallics*, 1987, **6**, 203 (*synth, cryst struct, ir, pmr, B-11 nmr*)

IC-004442

$C_4H_{20}B_4N_2$

Bis(μ-dimethylamino)tetraborane(10)

[108083-02-9]



M 139.4

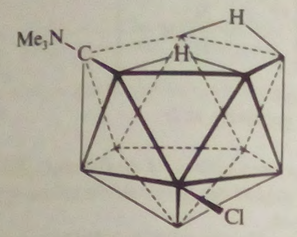
Air-sensitive clear liq. Sol. CH_2Cl_2. Mp −4° to −3°. Stable when neat, dec. slowly in soln.

Gaines, D.F. *et al, Inorg. Chem.*, 1988, **27**, 1839 (*synth, ir, pmr, B-11 nmr, ms*)

IC-004443

$C_4H_{20}B_{10}ClN$

4-Chloro-7-trimethylamine-7-carbaundecaborane(14)



M 225.7

nido-. Colourless solid. Sol. CH_2Cl_2, MeCN.

Khan, S.A. *et al, J. Chem. Soc., Dalton Trans.*, 1990, 2503 (*synth, pmr, B-11 nmr, ms*)

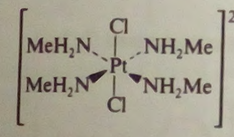
IC-004444

$C_4H_{20}Cl_2N_4Pt^{2\oplus}$

Dichlorotetrakis(methylamine)platinum(*IV*)(2+), 8CI

Dichlorotetrakis(methanamine)platinum(2+), 9CI

[21430-86-4]



M 390.2 (ion)

***trans*-form** [29484-86-4]

Dichloride: [49815-97-6].

$C_4H_{20}Cl_4N_4Pt$ M 461.1

Yellow solid. Sol. Me_2CO.

Tetrakis(methylamine)platinum(2+) double salt, tetraperchlorate: [102533-49-3].

$C_8H_{40}Cl_6N_8O_8Pt_2$ M 979.3

Yellow-orange or orange-red solid. Has stacked structure and mixed-valence properties.

[53406-73-8]

Inorg. Synth., 1974, **15**, 93 (*synth*)

Clark, R.J.H., *J. Chem. Soc., Dalton Trans.*, 1986, 403 (*synth, struct, uv, raman*)

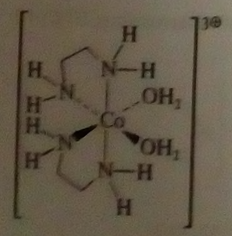
IC-004445

$C_4H_{20}CoN_4O_2^{3\oplus}$

Diaquabis(ethylenediamine)cobalt(*III*)(3+)

Bis(ethylenediamine)diaquacobalt(III)(3+)

[21242-06-8]



Λ-cis-form

M 215.1 (ion)

Octahedral. Subject of many kinetic studies on substitutions. Other salts known.

Λ-cis-form [18485-07-9]

Trinitrate: Red cryst. $[\alpha]_{546.1}$ −300°.

(±)-cis-form [21247-59-6]

Trinitrate: [16300-52-0].

Red.

trans-form [23523-26-4]

Trinitrate: [17967-05-4].

[18660-77-0]

Dwyer, F.P., *J. Am. Chem. Soc.*, 1963, **85**, 1215 (*synth*)

Brown, P.H. *et al, Inorg. Chem.*, 1968, **7**, 1872 (*kinetics*)

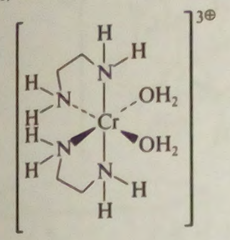
van Eldik, R., *Inorg. Chem.*, 1979, **18**, 1997 (*kinetics*)

IC-004446

$C_4H_{20}CrN_4O_2^{3\oplus}$

Diaquabis(ethylenediamine)chromium(*III*)(3+), 8CI

Diaquabis(1,2-ethanediamine-N,N′)chromium(III)(3+), 11CI, 10CI, 9CI



Λ,cis-form

M 208.2 (ion)

Octahedral cation.

Λ, cis-form

(+)-form

Config. determined by cd. Obt. in soln; not isol.

(±),cis-form [22432-36-6]

Tribromide: [15040-49-0].

Light-sensitive, orange cryst. $+2H_2O$ (HBr). In acidified soln, slowly converts to mixt. of *cis* and *trans* forms.

trans-form [17993-12-3]

Trichloride: [33849-41-1].

Cryst. $+ 1H_2O$.

Tribromide: Lustrous orange cryst. (aq. HBr).

Triperchlorate: [74929-62-7].

Solid $+ 2H_2O$. Sol. aq. Py.

Bis(ethylenediamine-N,N′)fluorohydroxychromium(1+), perchlorate: see *Bis(ethylenediamine) fluorohydroxychromium*(III)(1+), *IC-004403*

[25884-85-9, 56846-55-0]

Dubicki, L. *et al, Inorg. Chem.*, 1971, **10**, 2043 (*uv-vis*)

Kindred, I.J. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 1359 (*resoln, ion, cd*)

Jackson, W.G. *et al, Inorg. Chim. Acta*, 1977, **22**, 111 (*synth, trans bromide*)

Inorg. Synth., 1978, **18**, 75 (*synth, cis bromide*)

Solans, X. *et al, Cryst. Struct. Commun.*, 1982, **11**, 1199 (*cryst struct*)

IC-004447

$C_4H_{20}MnN_2O_6P_2^{2\oplus}$

Diaquabis[α-aminomethyl(methyl)phosphonic acid] manganese(2+)

Bis[(aminomethyl)methylphosphinato-O] diaquamanganese(6+) tetrahydrogen

$[Mn[OP(O)MeCH_2NH_3]_2(OH_2)_2]^{2\oplus}$

M 309.0 (ion)

Polymeric: *cis*-octahedral at Mn with bridging phosphonic acid groups (MnOPOMn links).

Dibromide: [64074-68-6].

Colourless prisms $+ 2H_2O$.

Glowiak, T. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 2648 (*cryst struct*)

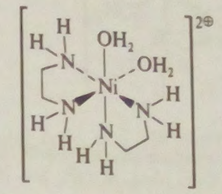
IC-004448

$C_4H_{20}N_4NiO_2^{2\oplus}$

Diaquabis(ethylenediamine)nickel(*II*)(2+), 8CI

Diaquabis(1,2-ethanediamine-N,N′)nickel(2+), 9CI

[15554-67-3]



cis-form

M 214.9 (ion)

Forms *cis* or *trans* struct. depending on anion.

cis-form

Bis-tetraphenylborate: [15747-93-0].

Purple solid. Sol. aq. EtOH. Mp 138° dec.

trans-form

Bis-tetrafluoroborate: [37488-18-9].

Violet cryst.

Diperchlorate: [15307-11-6].

Blue-violet cryst. Sol. H_2O.

▷ Potentially explosive.

[15686-01-8, 19332-81-1, 45838-76-4]

Farago, M.E. *et al, J. Chem. Soc. A*, 1967, 820 (*synth, ir, uv-vis, magnetism*)

Tomlinson, A.A.G. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1671 (*synth, ir, uv-vis*)

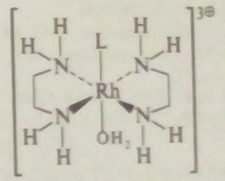
Minacheva, L.Kh. *et al, Russ. J. Struct. Chem.* (*Engl. Transl.*), 1974, **15**, 408 (*cryst struct*)

IC-004449

$C_4H_{20}N_4O_2Rh^{3\oplus}$

Diaquabis(ethylenediamine)rhodium(*III*)(3+)

Diaquabis(1,2-ethanediamine-N,N′)rhodium(III)(3+), 9CI



L = H_2O

M 259.1 (ion)

Octahedral.

trans-form

Triperchlorate: [41188-56-1].

Pale yellow cryst. Sol. H_2O.

▷ Potentially explosive.

Burgess, C., *Inorg. Chim. Acta*, 1975, **13**, 35 (*ir, uv, raman*)

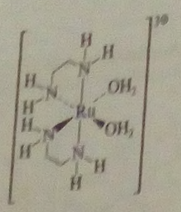
IC-004450

$C_4H_{20}N_4O_2Ru^{3\oplus}$

Diaquabis(ethylenediamine)ruthenium(*III*)(3+)

Diaquabis(1,2-ethanediamine-N,N')ruthenium(III)(3+), 10Cl

[55870-36-5]



M 257.2 (ion)

Prepd. by the hydration of eg. Aquachlorobis(ethylenediamine)ruthenium(*III*)(2+), IC-004413 in H_2O. Only obsd. in soln. Sol. H_2O. Readily undergoes anation.

Broomhead, J.A. *et al*, *J. Chem. Soc. A*, 1967, 546 (*synth, uv*)
Broomhead, J.A. *et al*, *Inorg. Chem.*, 1971, **10**, 85 (*anation*)
Poon, C.-K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 128 (*electrochem*)

IC-004451

$C_4H_{20}N_4Pt^{2\oplus}$

Tetrakis(methylamine)platinum(*II*), 8Cl

Tetrakis(methanamine)platinum(2+), 9Cl

[21430-91-1]

$[Pt(NH_2Me)_4]^{2\oplus}$

M 319.3 (ion)

Square planar struct. Synth. from *cis*-$[Pt(DMSO)_2Cl_2]$ + $MeNH_2$.

Dichloride: [15273-29-7].
$C_4H_{20}Cl_2N_4Pt$ M 390.2
White solid. Sol. H_2O.

Tetrachloroplatinate: [14160-32-4].
$C_4H_{20}Cl_4N_4Pt_2$ M 656.2
Green needles. Sol. H_2O. Has linear chain struct.

Dichlorotetrakis(methylamine)platinum(IV) double salt, tetraperchlorate: see *Dichlorotetrakis(methylamine)platinum(IV)(2+), IC-004444*

Watt, G.W. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2007 (*synth, ir*)
Cradwick, M.E. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 446 (*struct*)
Kukushkin, Yu.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 595 (*synth*)

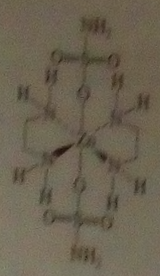
IC-004452

$C_4H_{20}N_4O_8S_2Zn$

Bis(ethylenediamine)bis(sulfamato-*O*)zinc

Bis(1,2-ethanediamine-N,N')bis(sulfamato-O)zinc, 9Cl

[57298-95-0]



M 377.7

trans-Octahedral molecule. Solid.

Hughes, M.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1478 (*synth, ir*)

IC-004453

$C_4H_{20}N_8O_6Zn^{2\oplus}$

Diaquatetrakis(urea-*O*)zinc(2+)

$[Zn(OH_2)_2[O{=}C(NH_2)_2]_4]^{2\oplus}$

M 341.6 (ion)

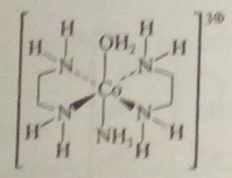
Diperchlorate: [59272-48-9].
Cryst. + $2H_2O$ (H_2O). Sol. H_2O with dec.; dihydrate loses $1H_2O$ at 70-100°.

Molchanov, Ya.Ya. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 476; 1977, **22**, 1760 (*synth, ir*)

IC-004454

$C_4H_{21}CoN_5O^{3\oplus}$

Ammineaquabis(ethylenediamine)cobalt(*III*)(3+), 8Cl



M 214.1 (ion)

trans-Octahedral.

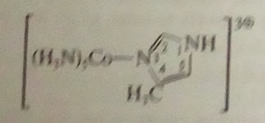
Tri-perchlorate: [33031-24-2].
Orange cryst. Sol. H_2O.
▷ Potentially explosive.

Lincoln, S.F. *et al*, *Inorg. Chem.*, 1971, **10**, 1254 (*synth*)

IC-004455

$C_4H_{21}CoN_7^{3\oplus}$

Pentaammine(4-methyl-1*H*-imidazole-N^3)cobalt(*III*)(3+), 1Cl



4-Methylimidazole-form

M 226.1 (ion)

Ligand coordination exhibits isomerism.

4-Methyl-1H-imidazole-form

Trichloride: [86568-74-3].
Yellow wool-like cryst. Sol. H_2O.

5-Methyl-1H-imidazole-form

Trichloride: [103203-21-0].
Deep yellow cryst. + $2H_2O$. Spar. sol. H_2O.

Hon, M.F. *et al*, *Inorg. Chem.*, 1983, **22**, 2693 (*synth, uv, pmr, kinetics*)
Henderson, W.W. *et al*, *Inorg. Chem.*, 1986, **25**, 3157 (*cryst struct, pmr, cmr*)

IC-004456

$C_4H_{21}N_5ORh^{3\oplus}$

Aquaamminebis(ethylenediamine)rhodium(*III*)(3+), 8Cl

Ammineaquabis(1,2-ethanediamine-N,N')rhodium(III)(3+), 10Cl

As Disquabis(ethylenediamine)rhodium(*III*)(3+), IC-004449 with

$L = NH_3$

M 258.1 (ion)

trans-form [15337-82-3]
Photochem. studied in soln.

Triperchlorate: Solid (conc. $HClO_4$). Sol. H_2O.
▷ Potentially explosive.

Trinitrate: Synth. by heating *trans*-$[Rh(en)_2Cl_2]NO_3$ with conc. aq. NH_3 and adding HNO_3. Sol. H_2O.

[61697-87-8, 70223-45-9]

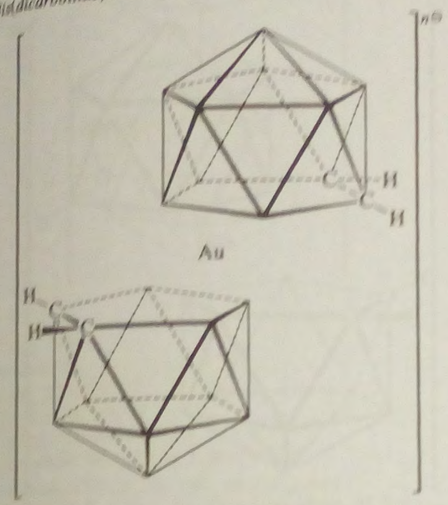
Pfe, A.J., *J. Chem. Soc. A*, 1970, 393 (*synth, uv*)

IC-004457

$C_4H_{22}AuB_{18}^{\ominus}$

Bis[undecahydro-1,2-dicarbaundecaborato(2−)]aurate(1−), 8Cl

Bis(dicarbollide)aurate(1−)



n = 1

M 461.7 (ion)
"Slipped" sandwich struct.

Et_4N salt: Glittering red plates (CH_2Cl_2/hexane). Sol. Me_2CO, CH_2Cl_2, MeCN.

$MePh_3P$ salt: Large red cryst. (CH_2Cl_2/hexane).

Warren, L.F. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 4823 (*synth, nmr, pmr, ir*)
Wing, R.M., *J. Am. Chem. Soc.*, 1968, **90**, 4828 (*cryst struct*)

IC-004458

$C_4H_{22}AuB_{18}^{2\ominus}$

Bis[undecahydro-1,2-dicarbaundecaborato(2−)]aurate(2−), 8Cl

Bis(dicarbollide)aurate(2−)

As Bis[undecahydro-1,2-dicarbaundecaborato(2−)]aurate(1−), IC-004457 with

n = 2

M 461.7 (ion)
"Slipped" sandwich struct.

Bis-Et_4N salt: Blue, paramagnetic microcryst. Sol. THF, MeCN. $\mu_{eff} = 1.79\mu_B$.

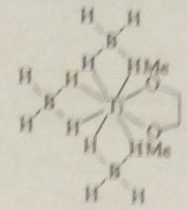
Warren, L.F. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 4823 (*synth*)

IC-004459

$C_4H_{22}B_2O_2Ti$

(1,2-Dimethoxyethane-*O,O'*)tris[tetrahydroborato(1−)-*H,H'*]titanium

[61735-11-3]



M 182.5
Borohydride deriv. with distorted trig. bipy. geometry around Ti. Precursor for chemical vapour deposition of TiB_2 film. Air-sensitive thermally-stable light-blue cryst. (Et_2O). Sol. Et_2O. Ir ν_{max} 2412, 2114 cm^{-1}. Paramagnetic, $\mu_{eff} = 1.8\mu_B$.

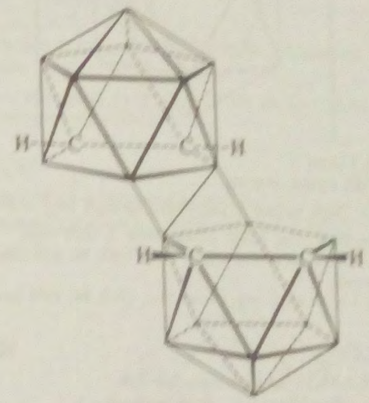
Jensen, J.A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 1643 (*synth, cryst struct, use, ir, auger spectrum*)

IC-004460

$C_4H_{22}B_{18}$

9,9-Bi-7,8-dicarbaundecaborane(12)

[55522-17-3]



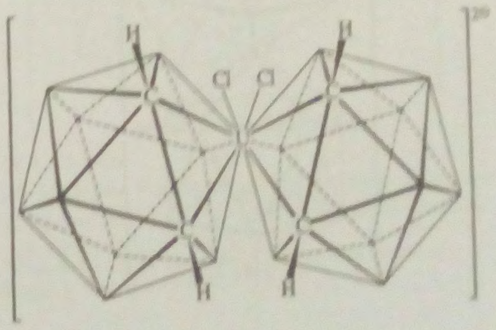
M 264.8
Synth. by oxidn. of the K salt of $7,8\text{-}C_2B_9H_{12}^{\ominus}$ with K_2CrO_4 in aq. H_2SO_4.

Hermanek, S. *et al*, *Collect. Czech. Chem. Commun.*, 1974, **39**, 2363 (*synth, B-11 nmr*)

IC-004461

$C_4H_{22}B_{18}Cl_2U^{2\ominus}$

Dichlorobis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]uranate(2−)



$C_4H_{22}B_{18}Co^{\ominus}$ – $C_4H_{22}B_{18}Cu^{2\ominus}$

M 573.7 (ion)
De-Li salt, octa-THF complex: [62339-85-9].
$C_{56}H_{86}B_{36}Cl_2Li_2O_8U$ M 1164.4
Yellow-orange cryst. Dec. by air and water.

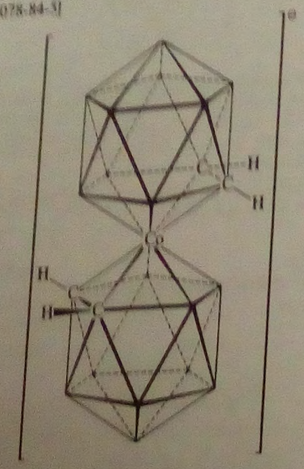
Francesk, F.R. *et al, J. Am. Chem. Soc.*, 1977, **99**, 1702 (*synth, ir, cryst struct*)

IC-004462

$C_4H_{22}B_{18}Co^{\ominus}$

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]cobaltate(1−)

[11078-84-3]



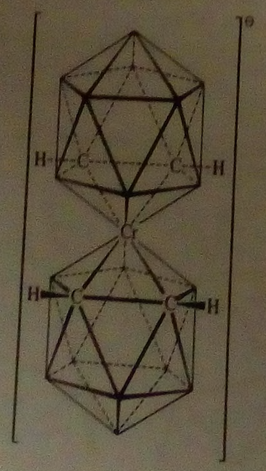
M 323.7 (ion)
Proposed struct. shown.
Cs salt: Dark yellow cryst. (Me_2CO aq.). Mp >300°.

De Boer, D.G. *et al, Inorg. Chem.*, 1968, **7**, 2288 (*use*)
Young, D.C. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, pmr, ir, uv-vis*)
Francis, J.N. *et al, J. Am. Chem. Soc.*, 1972, **94**, 4878 (*use*)

$C_4H_{22}B_{18}Cr^{\ominus}$ IC-004463

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]chromate(1−)

[80818-58-2]



M 316.8 (ion)
Cs salt: [12373-83-0].
Air-stable, dark violet cryst. (H_2O). $\mu_{eff} = 3.85\mu_B$. Thermally stable to 280°.

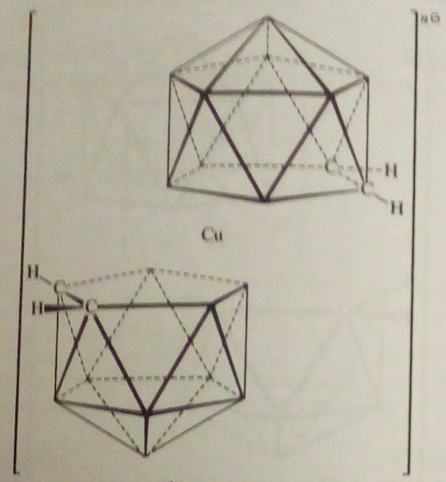
Ruble, H.W. *et al, Inorg. Chem.*, 1968, **7**, 2279 (*synth, ir, uv-vis*)
Crawford, V.H. *et al, Inorg. Chem.*, 1979, **18**, 1600 (*electronic progs*)

$C_4H_{22}B_{18}Cu^{\ominus}$ IC-004464

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]cuprate(1−), 9CI

Bis(dicarbollide)cuprate(1−)

[51805-68-6]



$n = 1$

M 328.3 (ion)
An example of a "slipped" sandwich complex.
$MePh_3P$ salt: Dark blood-red cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2, Me_2CO.

Warren, L.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4823 (*synth*)
Wing, R.M. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4828 (*cryst struct*)
Mingos, D.M.P. *et al, J. Organomet. Chem.*, 1978, **146**, C37.

$C_4H_{22}B_{18}Cu^{2\ominus}$ IC-004465

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]cuprate(2−), 9CI

Bis(dicarbollide)cuprate(2−)

As Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]cuprate(1−), IC-004464 with

$n = 2$

M 328.3 (ion)
An example of a "slipped" sandwich complex.
Di-K salt: [42992-84-7].
Blue cryst. (Me_2CO/hexane). Sol. CH_2Cl_2, Me_2CO.
Bis-Et_4N salt: [11072-22-3].
Dark royal blue platelets (Me_2CO/hexane). Sol. Me_2CO; insol. heptane.

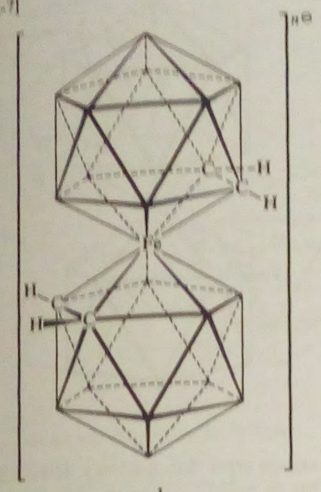
Wing, R.M., *J. Am. Chem. Soc.*, 1967, **89**, 5599 (*cryst struct*)
Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth*)
Warren, L.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4823 (*synth*)
Mingos, D.M.P. *et al, J. Organomet. Chem.*, 1978, **146**, C37.

$C_4H_{22}B_{18}Fe^{\ominus}$ IC-004466

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]ferrate(1−)

Bis-π-(3)-1,2-Dicarbollyliron(1−)

[63465-56-7]



$n = 1$

M 320.6 (ion)
Paramagnetic.
Cs salt: [12304-97-1].
Black cryst. (H_2O).
Me_4N salt: [12304-95-9].
Red plates (Me_2CO aq.). Mp >300°.

Inorg. Synth., 1967, **10**, 91; 1970, **10**, 111 (*synth*)
Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, ir, uv, nmr*)
Birchall, T. *et al, Inorg. Chem.*, 1971, **10**, 399 (*mössbauer*)
Wiersema, R.J. *et al, J. Am. Chem. Soc.*, 1974, **96**, 761 (*cmr, nmr*)
Ammeter, J.H., *J. Magn. Reson.*, 1978, **30**, 299 (*esr*)

$C_4H_{22}B_{18}Fe^{2\ominus}$ IC-004467

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]ferrate(2−)

Bis-π-(3)-1,2-dicarbollyliron(2−)

[51868-94-1]

As Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]ferrate(1−), IC-004466 with

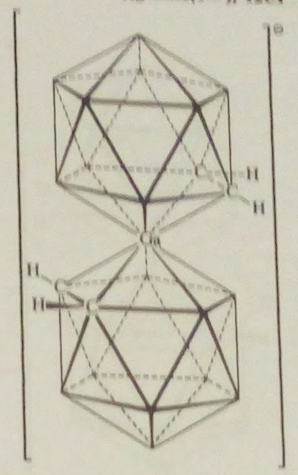
$n = 2$

M 320.6 (ion)
Diamagnetic.
Bis-Me_4N salt: Deep-pink cryst. (Me_2CO/toluene).

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, ir, pmr, nmr, uv*)

$C_4H_{22}B_{18}Ga^{\ominus}$ IC-004468

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]gallate(1−), 12CI



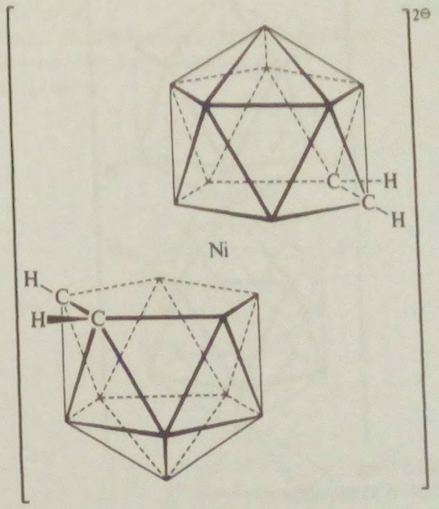
M 334.5 (ion)
commo-.
Tl(I) salt: [119769-33-4].
$C_4H_{22}B_{18}GaTl$ M 538.9
Colourless cryst. (toluene/heptane). Sol. toluene; insol. heptane.

Bandman, M.A. *et al, Inorg. Chem.*, 1989, **28**, 1204 (*synth, ir, pmr, B-11 nmr, ms, cryst struct*)

$C_4H_{22}B_{18}Ni^{2\ominus}$ IC-004469

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]nickelate(2−), 9CI

[36733-09-2]



M 323.5 (ion)
Bis-Me_4N salt: Pale-brown needles. Extremely air-sensitive.

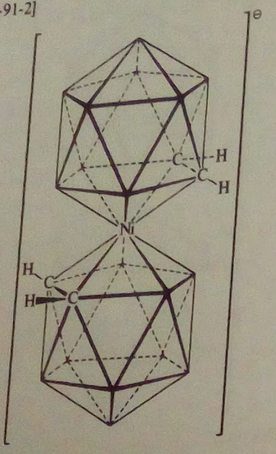
Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, ir, pmr*)
Wing, R.M., *J. Am. Chem. Soc.*, 1968, **90**, 4828 (*struct*)
Pavlik, I. *et al, CA*, 1976, **85**, 93221 (*pe*)

IC-004470

$C_4H_{22}B_{18}Ni^{\ominus}$

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]nickelate(1−), 9CI

[51159-91-2]



M 323.5 (ion)

Rb salt: Green-black lustrous cryst.

Me_4N salt: [51159-92-3].
Yellow-brown solid. Mp >300°.

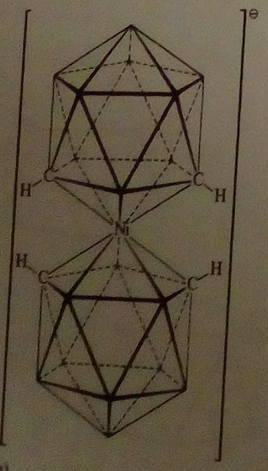
Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, ir, pmr*)

Hansen, F.V. *et al, Acta Chem. Scand.*, 1973, **27**, 1210 (*struct*)

IC-004471

$C_4H_{22}B_{18}Ni^{\ominus}$

Bis[(7,8,9,10,11-η)-undecahydro-7,9-dicarbaundecaborato(2−)]nickelate(1−), 9CI



M 323.5 (ion)
Postulated struct. shown.

Rb salt: [42443-78-7].
No phys. details recorded.

Me_4N salt: Olive-green cryst. (Me_2CO aq.). Mp >300°.

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 862, 879 (*synth, ir, pmr*)

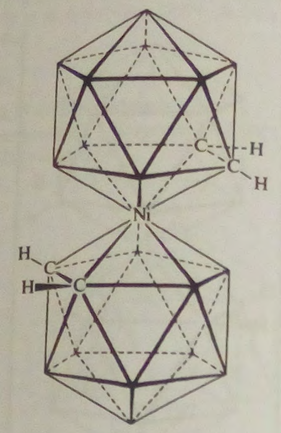
Pont, L.O. *et al, Inorg. Chem.*, 1974, **13**, 483 (*pe*)

IC-004472

$C_4H_{22}B_{18}Ni$

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]nickel, 9CI

[36548-57-7]



M 323.5
Air-stable orange cryst. Sol. most org. solvs. Subl. 150° *in vacuo*. Dec. at ~265°.

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, ir, pmr*)

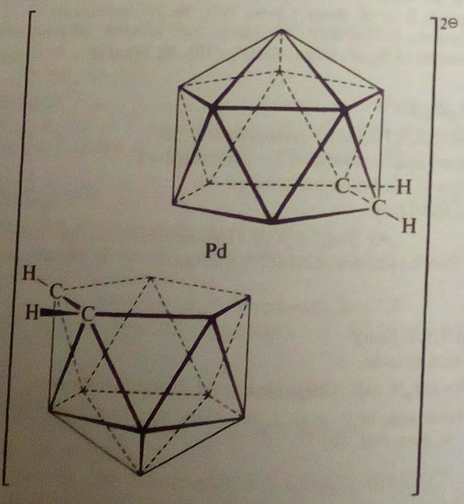
St Clair, D. *et al, J. Am. Chem. Soc.*, 1970, **92**, 1173 (*struct*)

Smith, D.E. *et al, J. Chem. Soc., Dalton Trans.*, 1971, 8 (*electrochem*)

IC-004473

$C_4H_{22}B_{18}Pd^{2\ominus}$

Bis[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]palladate(2−)



M 371.2 (ion)
Proposed 'slipped sandwich' struct. shown. From $Pd(acac)_2$ in glyme and soln. of $[1,2\text{-}B_9C_2H_{11}]^{2\ominus}$. Solns. dec. to Pd metal.

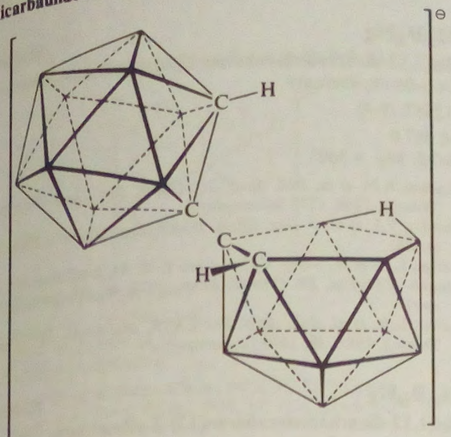
Bis-Et_4N salt: Air-sensitive, red-brown solid (Me_2CO/heptane). Diamagnetic.

Warren, L.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4823 (*synth, ir, B-11 nmr, electrochem*)

IC-004474

$C_4H_{22}B_{19}^{\ominus}$

7-[1′,2′-Dicarbadodecaboran-1′-yl]-dodecahydro-7,8-dicarbaundecaborate(1−)



M 275.6 (ion)
nido-closo-. Possesses anti-bacterial activity.

Tl(I) salt: [12603-29-1].
White cryst. ($HOAc/C_6H_6$).

Hawthorne, M.F. *et al, U.S. Govt. Res. Develop. Rep.*, 1970, **70**, 57 (*synth*)

Totani, T. *et al, J. Med. Chem.*, 1981, **24**, 1492 (*pharmacol*)

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1984, **106**, 2979 (*Tl salt, synth, derivs*)

Serino, A.J. *et al, J. Chromatogr.*, 1984, **291**, 384 (*chromatog, Me_4N salt*)

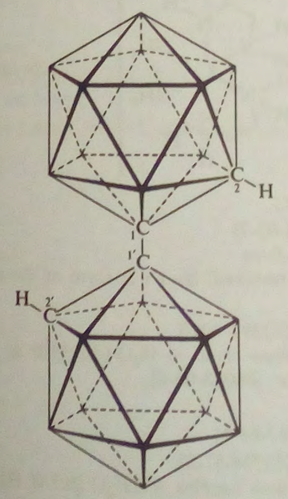
IC-004475

$C_4H_{22}B_{20}$

1,1′-Bi-1,2-dicarbadodecaborane(12)

1-[1′,2′-Dicarbadodecaboran-1′-yl]-1,2-dicarbadodecaborane(12)

[12075-02-4]



M 286.4
Synth. from $B_{10}H_{12}.2SEt_2$ and diacetylene in toluene at −25° or 80°. Cryst. Sol. C_6H_6.

Hawthorne, M.F. *et al, Inorg. Chem.*, 1973, **12**, 708 (*synth*)

Zakharkin, L.I. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1973, 1428; 1977, 2337 (*synth, raman, ir*)

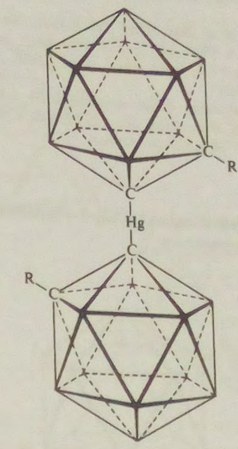
IC-004476

$C_4H_{22}B_{20}Hg$

Bis(1,2-dicarbadodecaboran(12)-1-yl)mercury

Di-o-carboranylmercury. Dibarenylmercury

[12364-82-8]



R = H

M 487.0
Solid. Does not melt up to 400°.

Zakharkin, L.I. *et al, J. Organomet. Chem.*, 1965, **4**, 211 (*synth*)

Stanko, V.I., *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1968, 414 (*electrochem*)

Denisovich, L.I. *et al, J. Organomet. Chem.*, 1973, **57**, 87 (*electrochem*)

Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)

Stanko, V.I. *et al, Zh. Obshch. Khim.*, 1978, **48**, 368 (*pmr, B-11 nmr*)

Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1981, **30**, 1670 (*ir, raman*)

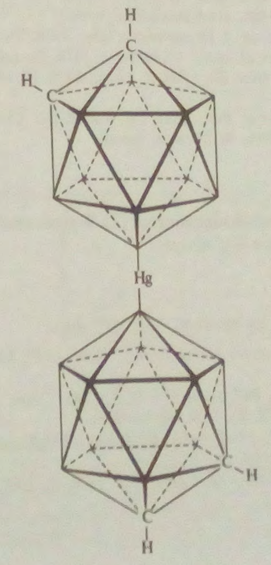
IC-004477

$C_4H_{22}B_{20}Hg$

Bis(1,2-dicarbadodecaboran(12)-9-yl)mercury

Di-o-carboran-9-ylmercury

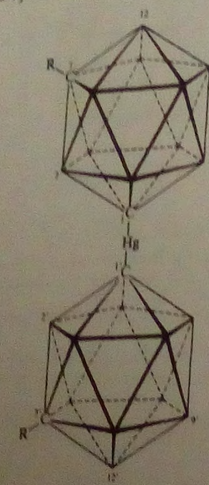
[64114-80-3]



M 487.0
Cryst. (C_6H_6). Mp 322-323°.
Bregadze, V.I. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1977, 1630 (*synth*)
Bregadze, V.I. *et al, J. Organomet. Chem.*, 1977, **136**, 281 (*synth, ir*)
Kampel', V.Ts. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1978, **27**, 1318 (*electrochem*)
Ol'dekop, Yu.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1978, **243**, 933 (*synth*)
Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1981, **30**, 1670 (*ir, raman*)

IC-004478

$C_4H_{22}B_{20}Hg$
Bis(1,7-dicarbadodecaboran(12)-1-yl)mercury
*Di-*m*-carboranylmercury*
[12364-83-9]



R = H

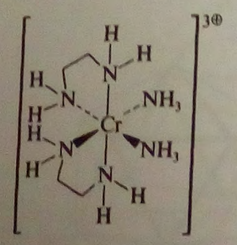
M 487.0
Cryst. (hexane). Mp >400°.
Stanko, V.I. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 414 (*electrochem, synth*)
Butin, K.P. *et al, J. Organomet. Chem.*, 1970, **25**, 11 (*electrochem*)
Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)
Stanko, V.I. *et al, Zh. Obshch. Khim.*, 1978, **42**, 368 (*pmr, B-11 nmr*)
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1981, **30**, 1670 (*ir, raman*)

$C_4H_{22}B_{20}Hg$ IC-004479
Bis(1,7-dicarbadodecaboran(12)-9-yl)mercury
*Di-*m*-carboran-9-ylmercury*
[64147-82-6]
M 487.0
Cryst. (C_6H_6 or hexane). Mp 350° dec.
Bregadze, V.I. *et al, J. Organomet. Chem.*, 1977, **136**, 281 (*synth, ir*)
Karpel', V.Ts., *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1978, **27**, 1318 (*electrochem*)
Ol'dekop, Yu.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1978, **243**, 933 (*synth*)
Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)
Zakharkin, L.I. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1979, **28**, 1750 (*synth*)
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1981, **30**, 1670 (*ir, raman*)

$C_4H_{22}B_{20}Hg$ IC-004480
Bis(1,12-dicarbadodecaboran(12)-1-yl)mercury
*Di-*p*-barenylmercury*
[12547-79-4]
M 487.0
Solid. Mp >360°.
Kashin, A.N. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1969, 1775 (*electrochem*)
Stanko, V.I. *et al, J. Gen. Chem. USSR (Engl. Transl.)*, 1969, 1857 (*synth*)
Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)
Stanko, V.I. *et al, Zh. Obshch. Khim.*, 1978, **48**, 368 (*pmr, B-11 nmr*)
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1981, **30**, 1670 (*ir, raman*)

$C_4H_{22}B_{20}Hg$ IC-004481
Bis(1,12-dicarbadodecaboran(12)-2-yl)mercury, 10CI
*Di-*p*-carboran-2-ylmercury*
[64156-80-5]
M 487.0
Cryst. (C_6H_6). Mp 323-325°.
Bregadze, V.I. *et al, J. Organomet. Chem.*, 1977, **136**, 281 (*synth*)
Kampel', V.Ts. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1978, **27**, 1318 (*electrochem*)
Leites, L.A. *et al, Inorg. Chim. Acta*, 1978, **31**, L467 (*raman*)
Leites, L.A. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1981, **30**, 1670 (*ir, raman*)

$C_4H_{22}CrN_6^{3\oplus}$ IC-004482
Diamminebis(ethylenediamine)chromium(*III*)(3+)
*Diamminebis(1,2-ethanediamine-*N,N′*)chromium*(III)(3+),*11CI, 10CI*

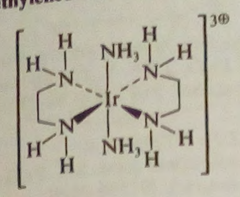


cis-form

M 206.2 (ion)
cis-form [66008-05-7]
More sol.-form
Has been resolved: the $(+)_D$ form of the anion has Λ-config.
Tribromide: [82794-80-7].
Orange-yellow cryst. + H_2O (dil. HBr at pH 1-2).
Triperchlorate: [66008-06-8].
Cryst.
trans-form [65982-64-1]
Tribromide: [82794-81-8].
Golden yellow needles + $2H_2O$ (0.1*M* HBr).
Triperchlorate: [65982-65-2].
Yellow plates + $1H_2O$ (0.1*M* HCl/$HClO_4$). H_2O of cryst. removed on heating at 50° for 1 h.
[82794-82-9, 82794-83-0]
Wong, C.F.C. *et al, Inorg. Chem.*, 1978, **17**, 1672 (*synth*)

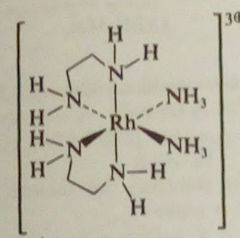
Shevchenko, Yu.N. *et al, Zh. Obshch. Khim.*, 1982, **52**, 1224; *J. Gen. Chem. USSR (Engl. Transl.)*, 1982, **52**, 1076 (*synth, ir, uv-vis*)
Kaizaki, S. *et al, Inorg. Chem.*, 1985, **24**, 2080 (*cd, cis-form, resoln*)

$C_4H_{22}IrN_6^{3\oplus}$ IC-004483
Diamminebis(ethylenediamine)iridium(*III*)(3+)



M 346.4 (ion)
trans-Octahedral geometry.
Triperchlorate: [65794-93-6].
White cryst. Sol. H_2O.
▷ Potentially explosive.
Weaver, T.R. *et al, Inorg. Chem.*, 1972, **11**, 2277 (*synth*)
Ogino, H. *et al, Inorg. Chem.*, 1978, **17**, 1118 (*synth, uv*)

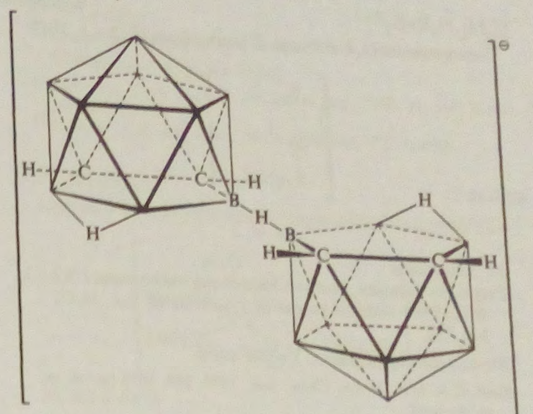
$C_4H_{22}N_6Rh^{3\oplus}$ IC-004484
Diamminebis(ethylenediamine)rhodium(*III*)(3+)
*Diamminebis(1,2-ethanediamine-*N,N′*)rhodium*(III)(3+), *10CI*
[65761-21-9]



cis-form

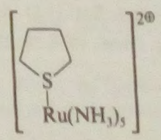
M 257.1 (ion)
cis-form
Major isomer.
Perchlorate: White cryst. Sol. H_2O.
▷ Potentially explosive.
Ogino, H., *Inorg. Chem.*, 1978, **17**, 1118 (*synth, pmr, ir, uv-vis*)

$C_4H_{23}B_{18}^{\ominus}$ IC-004485
9,9′-μ-Hydrobis[undecahydro-7,8-dicarbaundecaborate](1−), 9CI
Tricosahydrotetracarbadocosaborate(1−)
[55522-18-4]



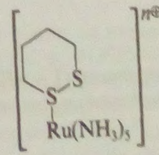
M 265.8 (ion)
K salt: Synth. by oxidn. of K salt of 7,8-$C_2B_9H_{12}$ with K_2CrO_4 in aq. H_2SO_4.
[39292-28-9]
Hermanek, S. *et al, Collect. Czech. Chem. Commun.*, 1974, **39**, 2363 (*synth, B-11 nmr*)

$C_4H_{23}N_5RuS^{2\oplus}$ IC-004486
Pentaammine(tetrahydrothiophene)ruthenium(*II*)(2+), 9CI
[58619-20-8]



M 274.3 (ion)
Pseudo-octahedral. Prepd. by treating Pentaammine(aqua) ruthenium(*II*)(2+), IC-019980 with tetrahydrothiophene. Sol. H_2O.
Bis-tetrafluoroborate: Yellow solid.
Kuehn, C.G. *et al, J. Am. Chem. Soc.*, 1976, **98**, 689 (*synth, ir, uv, pmr, raman, electrochem*)

$C_4H_{23}N_5RuS_2^{2\oplus}$ IC-004487
Pentaammine(1,2-dithiane-*S*^{1})ruthenium(*II*)(2+)



n = 2

M 306.4 (ion)
Pseudo-octahedral. Prepd. by treating Pentaammine(aqua) ruthenium(*II*)(2+), IC-019980 with an excess of 1,2-dithiane, or by stoichiometric oxidation of Pentaammine(butane-4-thiol-1-thiolato-*S*^{1})ruthenium(*III*)(2+), IC-004499 with Ce(*IV*). Sol. H_2O, Me_2CO.

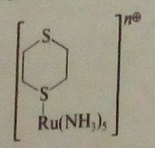
Bis-hexafluorophosphate: [70288-18-5].
Yellow salt.

Stein, C.A. *et al, Inorg. Chem.*, 1979, **18**, 2212 (*synth, uv, electrochem reaction*)

IC-004488

$C_4H_{23}N_5RuS_2^{2\oplus}$

Pentaammine(1,4-dithiane-S^1)ruthenium(*II*)(2+), 10CI



$n = 2$

M 306.4 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with an excess of 1,4-dithiane. Sol. H_2O, Me_2CO.

Bis-hexafluorophosphate: Yellow solid.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electochem*)

$C_4H_{23}N_5RuS_2^{3\oplus}$ **IC-004489**

Pentaammine(1,2-dithiane-S^1)ruthenium(*III*)(3+)

Pentaammine(tetramethylene disulfide-S)ruthenium(III)(3+)
[70288-19-6]

As Pentaammine(1,2-dithiane-S^1)ruthenium(*II*)(2+), IC-004487 with

$n = 3$

M 306.4 (ion)
pseudo-Octahedral. Prepd. by oxidizing Pentaammine(1,2-dithiane-S^1)ruthenium(*II*)(2+), IC-004487 with Ce(*IV*). Not isol. in solid state. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, Inorg. Chem.*, 1979, **18**, 2212 (*synth, uv, electrochem*)

$C_4H_{23}N_5RuS_2^{3\oplus}$ **IC-004490**

Pentaammine(1,4-dithiane-S^1)ruthenium(*III*)(3+), 10CI
[66083-96-3]

As Pentaammine(1,4-dithiane-S^1)ruthenium(*II*)(2+), IC-004488 with

$n = 3$

M 306.4 (ion)
Prepd. by oxidation of the Ru(*II*) analogue with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electrochem*)

$C_4H_{24}B_4Np$ **IC-004491**

Tetrakis[trihydromethylborato(1−)-*H*,*H*′,*H*″]neptunium
Tetrakis(methyltrihydroborato)neptunium
[86217-21-2]

$Np(BH_3Me)_4$

M 352.5
V. air- and moisture-sensitive dark-green cryst. Sol. PhCl. Subl. *in vacuo* at r.t.

Shinomoto, T. *et al, Inorg. Chem.*, 1983, **22**, 2351 (*synth, cryst struct*)

$C_4H_{24}B_4Th$ **IC-004492**

Tetrakis[trihydromethylborato(1−)-*H*,*H*′,*H*″]thorium, 11CI
Tetrakis(methyltrihydroborato)thorium(IV)
[86238-35-9]

$Th(BH_3Me)_4$

M 347.5
Most volatile thorium compd. known. Forms dimeric adducts with Et_2O, THF. V. air- and moisture-sensitive colourless cryst. Sol. PhCl. Mp 62-63°. Subl. 40° *in vacuo*.

Et_2O complex (2:1): [97295-99-3].
Air-sensitive colourless cryst. Sol. Et_2O. Mp 92-93°.
THF complex (dimeric): [97296-00-9].
$C_{16}H_{64}B_8O_2Th_2$ M 839.2
Air-sensitive colourless cryst. Sol. THF. Mp 112-114°. Subl. 100° *in vacuo*.

Shinomoto, R. *et al, Inorg. Chem.*, 1983, **22**, 2351; 1985, **24**, 2896 (*synth, nmr, ir, cryst struct, derivs*)
Beach, D.B. *et al, Inorg. Chem.*, 1986, **25**, 1735 (*pe*)
Green, J.C. *et al, Inorg. Chem.*, 1986, **25**, 2719 (*pe*)

$C_4H_{24}B_4U$ **IC-004493**

Tetrakis[trihydromethylborato(1−)-*H*,*H*′,*H*″]uranium, 11CI
Tetrakis(methyltrihydroborato)uranium
[86217-20-1]

$U(BH_3Me)_4$

M 353.5
V. air- and moisture-sensitive violet cryst. Sol. PhCl. Mp 72-74°. Subl. 50° *in vacuo*.

Dimethoxyethane complex: [97201-93-9].
$C_8H_{34}B_4O_2U$ M 443.6
Blue-green cryst. (toluene). Sol. toluene. Mp 141-142° dec. Subl. 125° *in vacuo*.

Schlesinger, H.I. *et al, J. Am. Chem. Soc.*, 1953, **75**, 222 (*synth*)
Shinomoto, T. *et al, Inorg. Chem.*, 1983, **22**, 2351; 1987, **26**, 2868 (*synth, ir, pmr, cryst struct, deriv*)

$C_4H_{24}B_4Zr$ **IC-004494**

Tetrakis[trihydromethylborato(1−)-*H*,*H*′,*H*″]zirconium(*IV*), 11CI
Tetrakis(methyltrihydroborato)zirconium(IV)
[86217-19-8]

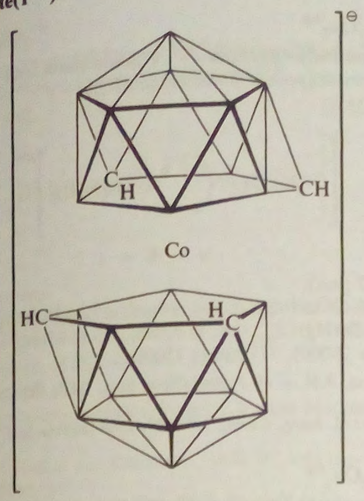
$Zr(BH_3Me)_4$

M 206.7
The four boron atoms are disposed tetrahedrally around the Zr and Zr—B—C is linear thus 12 hydrogens are in close contact with Zr. Synth. by reaction of $ZrCl_4$ with $LiBH_3Me$. Colourless solid. Sol. PhCl, Et_2O, THF. Mp 90-92°. Subl. 50° *in vacuo*. Has been used to form dilute crystals of actinide analogues.

Shinomoto, R. *et al, Inorg. Chem.*, 1983, **22**, 2351 (*cryst struct, ir, pmr*)
Gamp, E. *et al, J. Chem. Phys.*, 1984, **80**, 5963 (*use*)
Green, J.C. *et al, Inorg. Chem.*, 1986, **25**, 2718 (*pe*)

$C_4H_{24}B_{20}Co^{\ominus}$ **IC-004495**

Bis[η^6-dodecahydrodicarbadodecaborato(2−)]cobaltate(1−)

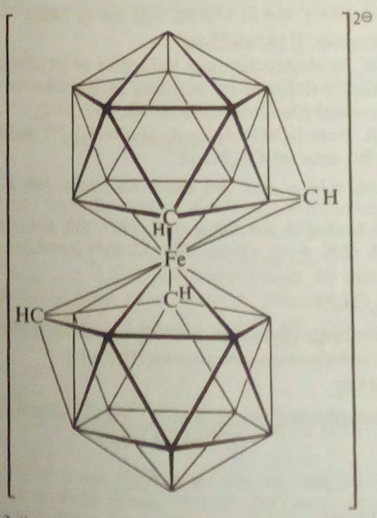


M 347.3 (ion)
Et_4N salt: Dark green cryst. Sol. CH_2Cl_2. Mp 230° dec. Rearranges on reflux in CH_2Cl_2.

Dustin, D. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1109 (*synth, B-11 nmr, pmr, ir, electrochem, uv-vis*)

$C_4H_{24}B_{20}Fe^{2\ominus}$ **IC-004496**

Bis[(7,8,9,10,11,12-η)-dodecahydro-7,9-dicarbadodecaborato(2−)]ferrate(2−), 9CI
Bis(π-$B_{10}C_2H_{12}$)ferrate(2−)
[55073-27-3]



M 344.3 (ion)
Bis-Et_4N salt: [40904-18-5].
Purple cryst. (Me_2CO/EtOH). Mp >240° dec.

Dustin, D.F. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1109 (*synth, polarog, pmr, nmr, ir, uv*)

$C_4H_{24}CoN_6O_2^{3\oplus}$ **IC-004497**

Pentaammine(ethyl glycinate)cobalt(*III*)(3+)
[73744-73-7]

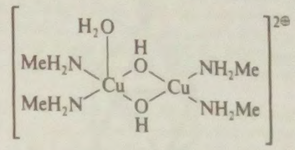
$[(H_3N)_5Co(H_2NCH_2COOEt)]^{3\oplus}$

M 247.2 (ion)
Tribromide: [26186-22-1].
Orange cryst. (dil. aq. HBr).

Buckingham, D.A. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3451 (*synth, pmr, uv, hydrol*)
Yeh, A. *et al, J. Am. Chem. Soc.*, 1980, **102**, 4725 (*synth*)

$C_4H_{24}Cu_2N_4O_3^{2\oplus}$ **IC-004498**

Aquadi-μ-hydroxytetrakis(methylamine)dicopper(*II*)(2+)



M 303.3 (ion)
Sulfate: Di-μ-hydroxobis[bis(methylamine)copper(II)] *sulfate monohydrate*
Dark blue cryst. Dec. in air.

Iitaka, Y. *et al, Acta Crystallogr.*, 1966, **20**, 803 (*synth, cryst struct*)

$C_4H_{24}N_5RuS_2^{2\oplus}$ **IC-004499**

Pentaammine(butane-4-thiol-1-thiolato-S^1)ruthenium(*III*)(2+)
Pentaammine(4-mercapto-1-butanethiolato)ruthenium(III)(2+)
[70288-20-9]

$[Ru(NH_3)_5S(CH_2)_4SH]^{2\oplus}$

M 307.4 (ion)
pseudo-Octahedral. Prepd. by the stoichiometric oxidation of Pentaammine(1,4-butanedithiol-*S*)ruthenium(*II*)(2+), IC-004500 with Ce(*IV*) or by aerial oxidation of Pentaammine(1,4-butanedithiol-*S*)ruthenium(*II*)(2+), IC-004500. Red soln.; not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, Inorg. Chem.*, 1979, **18**, 2212 (*synth, uv, electrochem*)

$C_4H_{25}N_5RuS_2^{2\oplus}$ **IC-004500**

Pentaammine(1,4-butanedithiol-*S*)ruthenium(*II*)(2+)
[70288-26-5]

$[Ru(NH_3)_5S(H)(CH_2)_4SH]^{2\oplus}$

M 308.4 (ion)
pseudo-Octahedral. Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with an excess of 1,4-butanedithiol or reducing Pentaammine(1,2-dithiane-S^1)ruthenium(*II*)(2+), IC-004487 with acidic Zn/Hg. Yellow soln.; not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, Inorg. Chem.*, 1979, **18**, 2212 (*synth, uv, electrochem*)

$C_4H_{28}B_{20}S_2$ IC-004501

Hexadecahydro-10,10'-bis[thiobis[methane]]-1,1'-bisdecaborane

Eicosaborane(16) compd. with thiobis[methane] (1:2), 9CI

[39436-10-7]

M 356.6

Obt. by electrol. of $(C_2H_5)_4N[1\text{-}B_{10}H_9SMe_2]$ in MeCN. Clear golden monoclinic cryst. (EtOH/MeCN).

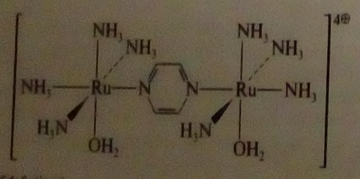
Schmitt, A.P. *et al, Inorg. Chem.*, 1974, **13**, 163 (*synth, ir, B-11 nmr, pmr*)

$C_4H_{32}N_{10}O_3Ru_2^{4\oplus}$ IC-004502

Octaamminediaqua-μ-(pyrazine-N^1:N^4)diruthenium(4+), 9CI

μ-Pyrazine-bis[tetraammine(aqua)ruthenium(II)]

[60184-05-6]



M 454.5 (ion)

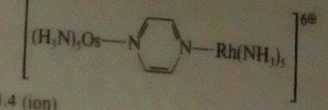
Prepd. by treating a mixt. of chloride salt of *cis*-Tetraamminedichlororuthenium(*III*)(1+), IC-016666 with $[V(OH_2)_6]^{2\oplus}$. A valuable reagent for the synth. of related dinuclear species. Prepd. in soln.; not isol. Sol. H_2O.

Creutz, C. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1086 (*synth, uv*)

$C_4H_{34}N_{12}OsRh^{6\oplus}$ IC-004503

Pentaammine(pentaamminerhodium)[μ-(1,4-pyrazine-N^1,N^4)]osmium(6+), 11Cl

[91230-43-2]



M 543.4 (ion)

Octahedral at both metals.

Hexachloride: Solid + $1H_2O$.

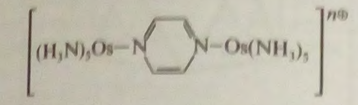
Magnuson, H. *et al, J. Am. Chem. Soc.*, 1983, **105**, 2507 (*synth, electrochem*)

$C_4H_{34}N_{12}Os_2^{4\oplus}$ IC-004504

Decaammine[μ-(pyrazine-N^1:N^4)]diosmium(*II*)(4+), 11Cl

μ-Pyrazinebis[pentaammineosmium(II)](4+)

[85282-25-3]



$n = 4$

M 630.7 (ion)

Not isol. as salt. Synth. by reduction of $[(Os(NH_3)_5)_2pz]^{6\oplus}$ with Zn(Hg). λ_{max} 247 (ε 7200), 275 (ε 2300), ~420(sh), 555 (ε 29000), 777 nm (ε 1100).

Magnuson, R.H. *et al, J. Am. Chem. Soc.*, 1983, **105**, 2507 (*uv, use*)

Lay, P. *et al, Inorg. Chem.*, 1988, **27**, 2364 (*electrochem, uv, use*)

$C_4H_{34}N_{12}Os_2^{5\oplus}$ IC-004505

Decaammine[μ-(pyrazine-N^1:N^4)]diosmium(*II,III*)(5+), 11Cl

μ-Pyrazinebis[pentaammineosmium(III,II)](5+)

[85282-23-1]

As Decaammine[μ-(pyrazine-N^1:N^4)]diosmium(*II*)(4+), IC-004504 with

$n = 5$

M 630.7 (ion)

Obt. from $[(NH_3)_5Os(OSO_2CF_3)](O_3SCF_3)_2$ by cation exchange chromatography, followed by spectrophotometric titration with $[Ru(NH_3)_6]^{2\oplus}$. λ_{max} 261 (ε 5000); 464 (ε 15000), 920 nm (ε 1300).

Pentabromide: [114595-25-4].

Synth. by electrochemical reduction of $[(Os(NH_3)_5)_2pz]^{6\oplus}$ in Me_2CO followed by addition of Et_4NBr.

Pentakis-methylbenzenesulfonate: [85282-24-2].

Synth. from $[(Os(NH_3)_5)_2pz]$, $[Ru(NH_3)_6]^{2\oplus}$ and the acid in a dil. soln. of CF_3SO_3H.

Magnuson, R.H. *et al, J. Am. Chem. Soc.*, 1983, **105**, 2507 (*synth, props*)

Dubicki, L. *et al, J. Am. Chem. Soc.*, 1985, **107**, 179 (*uv, ir*)

Lay, P.A. *et al, Inorg. Chem.*, 1988, **27**, 2364 (*synth, uv*)

$C_4H_{34}N_{12}Os_2^{6\oplus}$ IC-004506

Decaammine[μ-(pyrazine-N^1:N^4)]diosmium(*III*)(6+)

μ-Pyrazinebis[pentaammineosmium(III)](6+)

[91230-45-4]

As Decaammine[μ-(pyrazine-N^1:N^4)]diosmium(*II*)(4+), IC-004504 with

$n = 6$

M 630.7 (ion)

Hexachloride: [85293-63-6].

Synth. by various methods, using $[Os(NH_3)_5(OSO_2CF_3)](CF_3SO_3)_2$ as the starting material. Dark brown cryst. + $2H_2O$ (4*M* HCl).

[98194-39-9]

Magnuson, R.H. *et al, J. Am. Chem. Soc.*, 1983, **105**, 2507 (*synth, uv*)

Dubicki, L. *et al, J. Phys. Chem.*, 1984, **88**, 3940 (*uv*)

Bino, A. *et al, Inorg. Chem.*, 1985, **24**, 3969 (*cryst struct*)

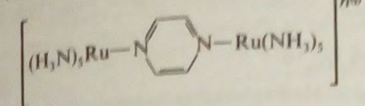
Lay, P.A. *et al, Inorg. Chem.*, 1988, **27**, 2364 (*synth, uv, electrochem*)

$C_4H_{34}N_{12}Ru_2^{4\oplus}$ IC-004507

Decaammine-μ-(pyrazine-N^1:N^4)diruthenium(4+), 9Cl

μ-Pyrazine-bis[pentaammineruthenium(II)]

[26253-76-9]



$n = 4$

M 452.5 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with pyrazine (Ru:pz = 2:1). Purple aq. soln.

Tetrabromide: [41557-48-6].

$C_4H_{34}Br_4N_{12}Ru_2$ M 772.1

Tetrakis(4-methylbenzenesulfonate): Purple needles + $1H_2O$.

Creutz, C. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1086 (*synth, uv, electrochem, ir*)

Citrin, P.H., *J. Am. Chem. Soc.*, 1973, **95**, 6472 (*pe*)

Strekas, T.C. *et al, Inorg. Chem.*, 1976, **15**, 974 (*raman*)

Bunker, B.C. *et al, J. Am. Chem. Soc.*, 1978, **100**, 3805 (*pmr*)

Lauher, J.W. *et al, Inorg. Chim. Acta*, 1980, **39**, 119 (*theory*)

Moore, K.J. *et al, Inorg. Chem.*, 1983, **22**, 1108 (*electrochem*)

Wong, K.J. *et al, Chem. Phys. Lett.*, 1986, **125**, 485 (*vibronic coupling*)

Fürholz, U. *et al, J. Phys. Chem.*, 1986, **90**, 3686 (*electron transfer*)

Joss, S. *et al, Inorg. Chem.*, 1989, **28**, 1815 (*mössbauer*)

Best, S.P. *et al, J. Am. Chem. Soc.*, 1989, **111**, 548 (*nir*)

$C_4H_{34}N_{12}Ru_2^{5\oplus}$ IC-004508

Decaammine-μ-(pyrazine-N^1:N^4)diruthenium(5+), 9Cl

μ-Pyrazine-bis[pentaammineruthenium(III,II)]. Creutz-Taube ion

[35599-57-6]

As Decaammine-μ-(pyrazine-N^1:N^4)diruthenium(4+), IC-004507 with

$n = 5$

M 452.5 (ion)

This ion has been the centre of a long controversy over whether it is a Class II or a Class III mixed-valence species. Ru—N_{pz} 200.6, Ru—$N_{NH_3\ transtopz}$ 212.7, Ru—$N_{NH_3\ cistopz}$ 212.2, 209.8 pm. Prepd. by oxidising Decaammine-μ-(pyrazine-N^1:N^4)diruthenium(4+), IC-004507 with Ag(*I*) or Ce(*IV*). Purple aq. soln. Sol. H_2O. $\mu_{eff} = 2.23\mu_B$.

Pentabromide: [41557-49-7].

$C_4H_{34}Br_5N_{12}Ru_2$ M 852.0

Pentakis-(4-methylbenzenesulfonate): Purple needles + $3H_2O$.

Creutz, C. *et al, J. Am. Chem. Soc.*, 1969, **91**, 3988 (*discovery*)

Elias, J.H. *et al, Inorg. Chem.*, 1972, **11**, 415 (*pmr, magnetism*)

Lim, H.S. *et al, Inorg. Chem.*, 1972, **11**, 1460 (*electrochem*)

Mayoh, B. *et al, J. Am. Chem. Soc.*, 1972, **94**, 2885 (*theory, classification*)

Creutz, C. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1086 (*synth, uv, nir, electrochem, ir*)

Citrin, P.H., *J. Am. Chem. Soc.*, 1973, **95**, 6472 (*pe*)

Srinivasan, V.S. *et al, J. Electrochem. Soc.*, 1973, **120**, 1359 (*electrochem*)

Mayoh, B. *et al, Inorg. Chem.*, 1974, **13**, 2273 (*theory, classification*)

Strekas, T.C. *et al, Inorg. Chem.*, 1976, **15**, 974 (*raman*)

Beattie, J.K. *et al, Inorg. Chem.*, 1976, **15**, 992 (*ir, pe*)

Cannon, R.D., *Chem. Phys. Lett.*, 1977, **49**, 299 (*nir*)

Callahan, R.W. *et al, J. Am. Chem. Soc.*, 1977, **99**, 1064 (*nir, theory*)

Beattie, J.K. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1121 (*cryst struct*)

Piepho, S.B. *et al, J. Am. Chem. Soc.*, 1978, **100**, 2996 (*theory*)

Bunker, B.C. *et al, J. Am. Chem. Soc.*, 1978, **100**, 3805 (*esr, pmr, magnetism*)

Hush, N.S. *et al, Chem. Phys. Lett.*, 1980, **69**, 128 (*esr*)

Krausz, E. *et al, Inorg. Chem.*, 1981, **20**, 434 (*ir*)

Tanner, M. *et al, Inorg. Chem.*, 1981, **20**, 2348 (*vibronic coupling*)

Citrin, P.H. *et al, J. Am. Chem. Soc.*, 1981, **103**, 3673 (*pe*)

Creutz, C., *Prog. Inorg. Chem.*, 1983, **30**, 1 (*rev*)

Richardson, D.E. *et al, Coord. Chem. Rev.*, 1984, **60**, 107 (*rev*)

Seddon, E.A. *et al, The Chemistry of Ruthenium*, Elsevier, Amsterdam, 1984, 315 (*rev*)

Fürholz, U. *et al, Inorg. Chem.*, 1985, **24**, 943 (*cryst struct*)

Creutz, C. *et al, Inorg. Chem.*, 1987, **26**, 2995 (*solvent effects*)

Winkler, J.R. *et al, J. Am. Chem. Soc.*, 1987, **109**, 2381 (*uv*)

Akhtar, M.J. *et al, Inorg. Chem.*, 1988, **27**, 1608 (*reaction*)

Isied, S.S. *et al, J. Am. Chem. Soc.*, 1988, **110**, 635 (*electron transfer*)

Joss, S. *et al, Inorg. Chem.*, 1989, **28**, 1815 (*mössbauer*)

Best, S.P. *et al, J. Am. Chem. Soc.*, 1989, **111**, 548 (*nir*)

Zhang, L.T. *et al, J. Phys. Chem.*, 1989, **93**, 3030 (*theory, uv*)

Piepho, S.B. *et al, J. Am. Chem. Soc.*, 1990, **112**, 4197 (*vibronic coupling*)

$C_4H_{34}N_{12}Ru_2^{6\oplus}$ IC-004509

Decaammine-μ-(pyrazine-N^1:N^4)diruthenium(6+)

μ-Pyrazine-bis[pentaammineruthenium(III)]

[38900-60-6]

As Decaammine-μ-(pyrazine-N^1:N^4)diruthenium(4+), IC-004507 with

$n = 6$

M 452.5 (ion)

Prepd. by oxidising corresp. (5+) ion with Ce(*IV*). Orange aq. soln.

Hexa-perchlorate: Orange cryst.

Creutz, C. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1086 (*synth, uv, electrochem, magnetism, ir*)

Citrin, P.H., *J. Am. Chem. Soc.*, 1973, **95**, 6472 (*pe*)

Srinivasan, V.S. *et al, J. Electrochem. Soc.*, 1973, **120**, 1359 (*electrochem*)

Strekas, T.C. *et al, Inorg. Chem.*, 1976, **15**, 974 (*raman*)

Bunker, B.C. *et al, J. Am. Chem. Soc.*, 1978, **100**, 3805 (*nmr, magnetism*)

Moore, K.J. *et al, Inorg. Chem.*, 1983, **22**, 1108 (*electrochem*)

Wong, K.P. *et al, Chem. Phys. Lett.*, 1986, **125**, 485 (*vibronic coupling*)

Fürholz, U. *et al, J. Phys. Chem.*, 1986, **90**, 3686 (*electron transfer*)

Creutz, C. *et al, Inorg. Chem.*, 1987, **26**, 2995 (*electrochem, uv*)

Joss, S. *et al, Inorg. Chem.*, 1989, **28**, 1815 (*mössbauer*)

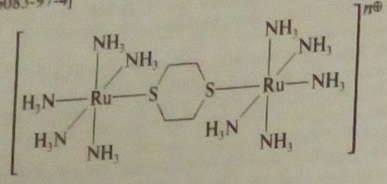
Best, S.P. *et al, J. Am. Chem. Soc.*, 1989, **111**, 548 (*nir*)

$C_4H_{38}N_{10}Ru_2S_2^{4\oplus}$ IC-004510

Decaammine[μ-(1,4-dithiane-S^1:S^4)]diruthenium(*II*)(4+),10Cl

μ-(1,4-Dithiane)bis[pentaammineruthenium(II)]

[66083-97-4]



$n = 4$

M 492.6 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with 1,4-dithiane stoicheiometrically. Sol. H_2O, Me_2CO.

Tetrakis-hexafluorophosphate: Yellow solid.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electrochem*)

$C_4H_{38}N_{10}Ru_2S_2^{5\oplus}$ IC-004511

Decaammine[μ-(1,4-dithiane-S^1:S^4)]diruthenium(5+), 10Cl

μ-(1,4-Dithiane)-bis[pentaammineruthenium(II,III)]

[66403-18-7]

As Decaammine[μ-(1,4-dithiane-S^1:S^4)]diruthenium(*II*) (4+),10Cl, IC-004510 with

$n = 5$

M 492.6 (ion)

Prepd. by oxidation of Decaammine[μ-(1,4-dithiane-S^1:S^4)] diruthenium(*II*)(4+),10Cl, IC-004510 with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

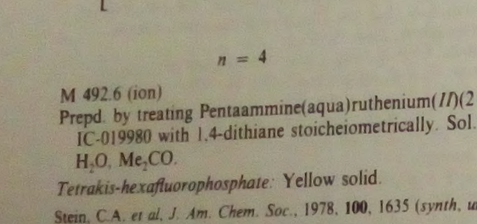
Stein, C.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electrochem*)

$C_4H_{46}N_{14}O_2Ru_3^{6\oplus}$ IC-004512

Decaamminebis(ethylenediamine)di-μ-oxotriruthenium(6+)

*Decaamminebis(1,2-ethanediamine-*N,N′*)di-μ-oxotriruthenium(6+), 9Cl. Bis[pentaammineruthenium*(III)-*μ-oxo]bis(1,2-diaminoethane)ruthenium*(IV)

[78005-14-8]



$n = 6$

M 625.7 (ion)

Commonly formulated as (*III, IV, III*), but the possibility of (*II, VI, II*) has been discussed. The struct. is staggered, by 45°. RuORu 177.2°, $Ru—O_{cent}$ 185, $Ru—O_{term}$ 189 pm. Prepd. by treating chloride salt of Ruthenium red with aq. ethylenediamine. Sol. H_2O.

Hexachloride: [36965-93-2].

$C_4H_{46}Cl_6N_{14}O_2Ru_3$ M 838.4

Green solid; red to transmitted light.

[36965-58-9]

Smith, P.M. *et al, Inorg. Chem.*, 1971, **10**, 1943 (*synth, cryst struct*)
Earley, J.E. *et al, Inorg. Chem.*, 1973, **12**, 323 (*uv, ir, theory, reactions*)
Campbell, J.R. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 2228 (*raman*)
Itabashi, M. *et al, Chem. Lett.*, 1981, 491 (*raman*)
Clark, R.J.H. *et al, Mol. Phys.*, 1981, **42**, 193 (*raman*)
Wagner, F.E. *et al, J. Chem. Soc., Dalton Trans.*, 1988, 1679 (*mössbauer*)

$C_4H_{46}N_{14}O_2Ru_3^{7\oplus}$ IC-004513

Decaamminebis(ethylenediamine)di-μ-oxotriruthenium(7+)

*Decaamminebis(1,2-ethanediamine-*N,N′*)di-μ-oxotriruthenium(7+), 9Cl. Bis[pentaammineruthenium*(IV)-*μ-oxo]bis(1,2-diaminoethane)ruthenium*(III)

As Decaamminebis(ethylenediamine)di-μ-oxotriruthenium(6+), IC-004512 with

$n = 7$

M 625.7 (ion)

Sol. H_2O.

Heptachloride: [36994-45-3].

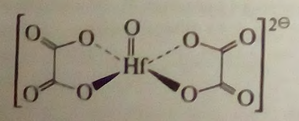
Prepd. by oxidising hexachloride salt of Decaamminebis(ethylenediamine)di-μ-oxotriruthenium(6+), IC-004512 with chlorine water. Brown cryst. + $5H_2O$.

Earley, J.E. *et al, Inorg. Chem.*, 1973, **12**, 323 (*synth, uv, ir, theory, reactions*)
Campbell, J.R. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 2228 (*raman*)
Clark, R.J.H. *et al, Mol. Phys.*, 1981, **42**, 193 (*raman*)
Wagner, F.E. *et al, J. Chem. Soc., Dalton Trans.*, 1988, 1679 (*mössbauer*)

$C_4HfO_9^{2\ominus}$ IC-004514

Dioxalato(oxo)hafnate(*IV*)(2−)

*Bis[ethanedioato(2−)-*O,O′*]oxohafnate*(IV)(2−), *11Cl*



M 370.5 (ion)

Synth. adding aq. oxalic acid to an aq. soln. of $HfCl_4$ followed by NH_3 or $MgCO_3$ and precipitating with EtOH.

Mg salt: [98262-33-0]. *Magnesium hafnyl oxalate* White solid + $7H_2O$. Thermal dec. → $MgHfO_3$.

Di-NH_4 salt: [93483-56-8]. *Ammonium hafnyl oxalate* White solid + $3H_2O$. Thermal dec. → pure HfO_2.

Zaitsev, L.M. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, **7**, 802 (*synth*)
Upor, E. *et al, Magy. Kem. Foly.*, 1971, **77**, 649; *CA*, **77**, 69672c (*soln extrn*)
Mittal, S. *et al, Thermochim. Acta*, 1985, **89**, 195 (*synth, thermal dec, ir*)

$C_4HgN_4^{2\ominus}$ IC-004515

Tetrakis(cyano-*C*)mercurate(2−)

Tetracyanomercurate(2−)

[19426-03-0]

$[Hg(CN)_4]^{2\ominus}$

M 304.6 (ion)

Di-K salt: [591-89-9].
Cryst. Low temp. form is ferroelastic with trigonal symmetry; high temp. form: spinel like.
▷ TT6230000.

Bis[potassium(dibenzo-18-crown-6)] complex: [112144-19-1].
Cryst. + $1H_2O$.

Di-Rb salt: [15634-25-0].
Cryst. Low temp.-form is ferroelastic; transforms to cubic spinel-like at 273K.

Ba salt, tetrakis-Py complex: [94553-89-6].
Cryst. Struct. contains 3D network of tetrahedral $Hg(CN)_4$ units; bridging CN. Ba coord. to 4 NC + 4 Py.

Bis(diphenyliodonium salt): [73012-26-7].
Cryst.

Bis-Ph_4P salt: [100765-78-4].
Cryst.

Bis-Ph_4As salt: [123118-46-7].
Cryst.

Li, Et_4N salt: [106633-51-6].
Cryst.

Cu(I), Et_4N salt: [106633-53-8].
Synth. from $[Et_4N]CN/CuCN/Hg(CN)_2$. Cryst.; exists in high- and low-temp. modifications. In both modifications, $Cu(NC)_4$ and $Hg(CN)_4$ tetrahedra are connected by Cu—NC—Hg bridges in 3D- cristobalite type struct. in which NEt_4 cations are located.

Chantry, G.W. *et al, J. Chem. Phys.*, 1961, **35**, 1037 (*raman, ion*)
Dehnicke, G. *et al, Ber. Bunsenges. Phys. Chem.*, 1974, **78**, 1010 (*ir, K salt*)
Haussuehl, S. *et al, Acta Crystallogr., Sect. C*, 1978, **34**, 968 (*low temp struct, Rb salt*)
Iwamoto, T. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 488 (*clathrates*)
Wasylishen, R.E. *et al, J. Magn. Reson.*, 1980, **41**, 341 (*nmr of ion*)
Sano, M. *et al, Bull. Chem. Soc. Jpn.*, 1981, **54**, 2023 (*pe, K salt*)
Kluefers, P. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1981, **156**, 255 (*cryst struct, Rb salt, nd*)
Wasylishen, R.E., *Can. J. Chem.*, 1982, **60**, 2194 (*cmr, K salt*)
Sano, M. *et al, Inorg. Chem.*, 1982, **21**, 2521 (*N-15 nmr, cmr, ion*)
Adams, D.M. *et al, J. Mol. Struct.*, 1982, **79**, 415 (*raman, phase trans, K salt*)
Gyoryova, K. *et al, Chem. Zvesti*, 1983, **37**, 773 (*synth, ir, Ph_2I salt*)
Albright, M.J. *et al, J. Organomet. Chem.*, 1983, **259**, 37 (*Hg-199 nmr*)
Brodersen, K. *et al, Z. Anorg. Allg. Chem.*, 1984, **516**, 30 (*synth, struct, Ba(Py)$_4$ salt*)
Earl, G.J. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 663 (*raman, ion*)
Gerlach, P.N. *et al, J. Chem. Phys.*, 1986, **85**, 604 (*cryst struct, thermal anal, raman, nmr*)
Thiele, G. *et al, Z. Naturforsch., B*, 1986, **41**, 1 (*synth, cryst struct, mixed Cu and Li salts*)
Grossmann, J. *et al, Thermochim. Acta*, 1987, **112**, 71 (*mixed Cu and Li salts*)
Mok, K.F., *Inorg. Chim. Acta*, 1988, **142**, 27 (*synth, ir, pmr bis(potassium dibenzo-18-crown-6) salt*)
Korpar-Coliq, B. *et al, Inorg. Chim. Acta*, 1988, **150**, 113 (*synth, Ph_4As and Ph_4P salt*)

$C_4HgN_4O_4^{2\ominus}$ IC-004516

Tetrakis(cyanato-*O*)mercurate(2−)

[26809-11-0]

$[Hg(OCN)_4]^{2\ominus}$

M 368.6 (ion)

Di-K salt: [28331-02-4].
Cryst.

Bis-Ph_4As salt: [15727-00-1].
White solid.

[15726-99-5]

Beck, W. *et al, Z. Anorg. Allg. Chem.*, 1966, **347**, 304 (*synth, ir*)
Tsintsadze, G.V. *et al, Soobshch. Akad. Nauk. Gruz. SSR*, 1969, **56**, 301 (*synth, ir, K salt*)
Katt, B. *et al, J. Electroanal. Chem. Interfacial Electrochem.*, 1970, **24**, 61 (*stability const*)
Golub, A.M. *et al, Tr. -Gruz. Politekh. Inst. im. V.I. Lenina*, 1970, 23 (*synth, ir, powder struct, K salt*)

$C_4HgN_4S_4^{2\ominus}$ IC-004517

Tetrakis(thiocyanato-*S*)mercurate(2−)

Tetrathiocyanatomercurate(2−)

[17845-33-9]

$[Hg(SCN)_4]^{2\ominus}$

M 432.9 (ion)

Di-K salt: [14099-12-8].
Cryst.

Di-K, bis-dibenzo-18-crown-6 complex, EtOH solvate: [120062-65-9].
Cryst.

K, bis(ethylenedithio)tetrathiafulvalene salt: [123341-38-8].
Metallic down to 1.5K. Cryst. Struct. comprises alternate stacks of 2D network of (BEDT-TTF) units and of $[KHg(SCN)_4]^{\ominus}$ anions.

Di-Rb salt: [52139-49-8].
Cryst.

Di-Cs salt: [29993-48-4].
Cryst.

Sr salt, trihydrate: [86525-95-3].
Cryst. Tetrahedral $Hg(SCN)_4$ and tricapped trigonal prismatic Sr (latter coord. to 4N + 5O).

Diaquacobalt(2+) salt, bis-2-pyrrolidinone complex: [110219-65-3].
Cryst. Struct. comprises polymeric chains of $[Hg(SCN)_4(H_2O)_2Co]$ with tetrahedral $Hg(SCN)_4$, octahedral Co [4*N*CS + $2OH_2$] and *trans* bridging CNS. 2-Pyrrolidinone groups are merely H-bonded to H_2O.

*Bis(dimethyl sulfoxide-*O*)cobalt(2+) salt:* [117355-43-8].
Cryst. Tetrahedral Hg and octahedral Co [2O (*trans*) + 4*N*CS].

Di-NH_4 salt: Cryst.

Lewis, J. *et al, J. Chem. Soc.*, 1961, 4590 (*ir, ion*)
Tramer, A. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1962, **59**, 232, 637 (*raman, ir, uv-vis, K, NH_4 salt*)
Tsivadze, A.Yu. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 2113 (*ir*)
Joergensen, C.K. *et al, Kgl. Dan. Vidensk. Selsk. Mata.-Fys. Medd.*, 1972, 38 (*pe*)
Larbot, A. *et al, Rev. Chim. Minér.*, 1973, **16**, 465 (*synth, ir*)
Asaji, T. *et al, Z. Naturforsch., B*, 1976, **31**, 1483 (*N-14 nqr, K salt*)
Kargol, J.A. *et al, Inorg. Chim. Acta*, 1977, **25**, L109 (*cmr, K salt*)
Persson, I. *et al, Acta Chem. Scand., Ser. A*, 1981, **35**, 295 (*soln struct, raman*)
Kirowa-Eisner, E. *et al, Anal. Chem.*, 1981, **53**, 581 (*stability const*)
Folkesson, B. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1982, **26**, 157 (*esca, K salt*)
Brodersen, K. *et al, Z. Anorg. Allg. Chem.*, 1983, **499**, 15 (*synth, cryst struct, Sr salt*)
Yamaguchi, T. *et al, Bull. Chem. Soc. Jpn.*, 1985, **58**, 3235 (*soln struct, raman, nmr*)
Ohtaki, H., *X-Sen Bunseku no Shinpo*, 1986, **18**, 157; *CA*, 1989, **111**, 69792 (*soln struct*)
Kinoshita, H. *et al, Bull. Chem. Soc. Jpn.*, 1987, **60**, 1933 (*synth, cryst struct, Co salt*)
Kinoshita, H. *et al, Bull. Chem. Soc. Jpn.*, 1988, **61**, 1169, 3350 (*synth, cryst struct, Co complexes*)
Mok, K.F. *et al, Acta Crystallogr., Sect. C*, 1989, **45**, 204 (*synth, cryst struct, K salt, di-benzo-18-c-6 complex*)
Oshima, M. *et al, Chem. Lett.*, 1989, 1159 (*synth, cryst struct, bedt-ttf deriv*)

$C_4HgN_4Se_4^{2\ominus}$ IC-004518

Tetrakis(selenocyanato-*Se*)mercurate(2−)

Tetraselenocyanatomercurate(2−)

[50937-28-5]

$[Hg(SeCN)_4]^{2\ominus}$

M 620.5 (ion)

Di-K salt: [15318-74-8].
Cryst.

Tetrakis(pyridine)strontium(2+) salt: [90580-32-8].
From $K_2Hg(SeCN)_4$ and $SrCl_2$ in MeOH, EtOH and Py. Cryst. Tetrahedral $Hg(SeCN)_4$: Sr 8-coord. (4 × *N*CSe + 4 × Py): bridging NCSe groups. Archimedean antiprismatic geometry.

Co(II) *salt:* Cryst. Tetrahedral $Hg(SeCN)_4$: tetrahedral Co.

[25930-46-5]

Frasson, E. *et al, Gazz. Chim. Ital.*, 1961, **91**, 750 (*synth, struct, Co salt*)
Tsintsadze, G.V. *et al, Soobshch. Akad. Nauk. Gruz. SSR*, 1966, **41**, 337 (*powder struct, Co, Zn and Cd salts*)
Tsintsadze, G.V. *et al, Tr. -Gruz. Politekh. Inst. im. V.I. Lenina*, 1967, 29, 53 (*cryst struct, Cd and Zn salts*)
Alasaniya, R.M. *et al, Tr. -Gruz. Politekh. Inst. im. V.I. Lenina*, 1967, 21; *CA*, 1968, **69**, 40772 (*synth, ir, powder struct, K salt*)
Kargol, J.A. *et al, Inorg. Chem.*, 1979, **18**, 2532 (*cmr, K salt*)
Pan, W.-H. *et al, Inorg. Chim. Acta*, 1980, **44**, L95 (*Se-77 nmr, K salt*)
Brodersen, K. *et al, Z. Naturforsch., B*, 1984, **39**, 582 (*synth, cryst struct, Sr salt*)

$C_4I_2N_4Pt^{2\ominus}$ IC-004519

Tetracyanodiiodoplatinate(*IV*)

Tetrakis(cyano-C)diiodoplatinate(2−)

[20756-59-6]

As Dibromotetrakis(cyano)platinate(2−), IC-003817 with

X = I

M 552.9 (ion)

Only *trans*-configuration known. Synth. from excess I_2 + $[Pt(CN)_4]^{2\ominus}$

trans-form

Di-K salt: [12075-15-9].
$C_4I_2K_2N_4Pt$ M 631.1
White cryst. Sol. H_2O, Me_2CO.

Bis-tetrabutylammonium salt: Golden-yellow cryst. Sol. Me_2CO.

[17176-69-1]

Poe, A.J. *et al, Inorg. Chim. Acta*, 1968, **2**, 159 (*synth*)
Brown, C. *et al, J. Organomet. Chem.*, 1977, **142**, 413 (*cmr, Pt-195 nmr*)
Osso, R. *et al, J. Coord. Chem.*, 1978, **8**, 169 (*synth, ir*)

$C_4I_2O_4Os$ IC-004520

Tetracarbonyldiiodoosmium

[17632-05-2]

As Dibromotetracarbonylosmium, IC-003818 with

X = Y = I

M 556.0

cis-form [17685-65-3]
Synth. from $Os_3(CO)_{12}$ and I_2 in C_6H_6 at 160° with 41 atm. CO. Yellow cryst. Ir 2165, 2086, 2101, 2050 cm^{-1}. Cmr CO_{ax} 159.2 ppm, CO_{eq} 156.4 ppm.

trans-form [25340-26-5]
Synth. from osmium oxyiodide with CO at 300 atm. and 60° in an autoclave. Yellow cryst. Ir ν_{CO} 2108 vw 2073 vs; ν_{MCO} 606.5 vs 585 s ν_{MC} 347 s cm^{-1}.

L'Eplattenier, F. *et al, Inorg. Chem.*, 1967, **6**, 2092 (*synth, ir*)
Hales, L.A.W. *et al, J. Chem. Soc. A*, 1967, 1389, 1932 (*synth, ir*)
Hales, L.A.W. *et al, Spectrochim. Acta*, 1967, **23**, 2981 (*ir*)
Pankowski, M. *et al, J. Organomet. Chem.*, 1969, **19**, 393 (*synth, ir*)
Vancea, L. *et al, J. Organomet. Chem.*, 1977, **134**, 219 (*synth, cmr*)

$C_4I_2MnO_4^{\ominus}$ IC-004521

Tetracarbonyldiiodomanganate(1−)

[37176-05-9]

As Dibromotetracarbonylmanganate(1−), IC-003816 with

X = I

M 420.7 (ion)

Me_4N salt: [53749-00-1].
Synth. from $MnI(CO)_5$ and $[Me_4N]I$ in diethyleneglycol dimethyl ether at 120°. Cryst.

Abel, E.W. *et al, J. Chem. Soc.*, 1964, 434 (*synth, ir, nmr*)
Ferona, M.F. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1814 (*props*)
Connor, J.A. *et al, J. Organomet. Chem.*, 1974, **73**, 351 (*props*)

$C_4InO_8^{\ominus}$ IC-004522

Bis(oxalato)indate(*III*)

Bis[ethanedioato(2−)-O,O′]indate(1−)

$[In(C_2O_4)_2]^{\ominus}$

M 290.8 (ion)

Na salt: [84934-62-3].
Colourless cryst. + $2H_2O$ (H_2O). Struct. comprises linked $In(C_2O_4)_4$ units with 8-coordinate In.

NH_4 salt: [84934-63-4].
White cryst. + $2H_2O$ (H_2O). Isomorph. with Na salt.

Kharitonov, Yu.Ya. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 460 (*ir*)
Dutt, N.K. *et al, Indian J. Chem., Sect. A*, 1976, **14**, 491 (*props*)
Bulc, N., *Acta Crystallogr., Sect. C*, 1983, **39**, 176 (*synth, cryst struct*)

$C_4In_2N_4$ IC-004523

Indium(1+) tetracyanoindate(1−)

Indium dicyanide. Indium(II) *cyanide (incorr.)*

$In[In(CN)_4]$

M 333.7

Synth. from HCN/H_2/In at 350°. White moisture-sensitive solid (subl.).

Goggin, P.L. *et al, J. Less-Common Met.*, 1966, **11**, 292 (*synth, ir, raman, props*)

$C_4Mg_2Na_6O_{16}S$ IC-004524

Tychite

Magnesium sodium carbonate sulfate ($Mg_2Na_6(CO_3)_4SO_4$)

[12188-92-0]

$Na_6Mg_2(CO_3)_4SO_4$

M 522.6

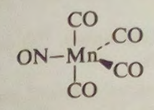
Mineral. Occurs assoc. with Northupite in California and Uganda. Cubic cryst.

Donnay, J.D.H. *et al, Crystal Data, Determinative Tables*, U.S. Dept. Commerce, NBS, JCPDS, Washington, USA, 3rd Ed., 1973, **2**, C-362 (*cryst struct*)
Pemberton, H.E., *Mineral. Rec.*, 1975, **6**, 74 (*rev*)
Zheng, M. *et al, CA*, 1982, **97**, 95666 (*ir*)

C_4MnNO_5 IC-004525

Tetracarbonylnitrosylmanganese, 8CI

[16104-17-9]



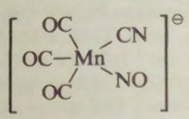
M 196.9

Synth. from $Na[Mn(CO)_5]$ and NOCl or from $HMn(CO)_5$ and *N*-methyl-*N*-nitroso-*p*-toluene-sulphonamide. Red liq. Mp −1.5°.

Treichel, P.M. *et al, J. Am. Chem. Soc.*, 1961, **83**, 2593 (*synth*)
Organomet. Synth., 1965, **1**, 164 (*synth*)
Waersik, H. *et al, Inorg. Chem.*, 1967, **6**, 1066.
Keeton, D.P. *et al, Inorg. Chim. Acta*, 1972, **6**, 33 (*props*)
Herberhold, M. *et al, J. Organomet. Chem.*, 1974, **67**, 81 (*props*)
Legzdins, P. *et al, Inorg. Chem.*, 1975, **14**, 1875 (*synth*)

$C_4MnN_2O_4^{\ominus}$ IC-004526

Tricarbonyl(cyano-*C*)nitrosylmanganate(1−)



M 194.9 (ion)

Na salt: [85962-27-2].
Synth. from $Mn(NO)(CO)_4$ and $NaN(SiMe_3)_2$ in C_6H_6 at 20°. Red-brown solid. Ir ν_{CN} 2110s; ν_{CO} 2010m, 1935s, 1907vs; ν_{NO} 1682s cm^{-1} (THF).

Bis(triphenylphosphine)iminium salt: [85962-29-4].
Red needles (1,2-dichloroethane/Et_2O). Mp 127° dec. Ir ν_{CN} 2107s; ν_{CO} 2020m, 1942s, 1912vs; ν_{NO} 1680s cm^{-1} (CH_2Cl_2).

Ph_4As salt: [85962-30-7].
Red needles (1,2-dichloroethane/Et_2O). Mp 123° dec. Ir ν_{CN} 2105s; ν_{CO} 2018s, 1942s, 1912vs; ν_{NO} 1680s cm^{-1} (CH_2Cl_2).

Moll, M. *et al, Z. Naturforsch., B*, 1983, **38**, 411 (*synth, ir*)

$C_4MnN_4O_4^{2\ominus}$ IC-004527

Tetrakis(cyanato-*N*)manganate(*II*)(2−), 9CI

Tetraisocyanatomanganate(II)(*2−*)

$[Mn(NCO)_4]^{2\ominus}$ (T_d)

M 223.0 (ion)

Bis-Et_4N salt: [14127-43-6].
Synth. from $[Et_4N][MnBr_4]$ and AgNCO in Me_2CO or $MeNO_2$. Pale green cryst. Sol. Me_2CO, $MeNO_2$. Mp 218°. μ_{eff} = 5.98μ_B (296K).

Forster, D. *et al, J. Chem. Soc.*, 1964, 2790; 1965, 262 (*synth, magnetism, uv, props, ir*)
Sabatini, A. *et al, Inorg. Chem.*, 1965, **4**, 959 (*props*)
Burmeister, J.L. *et al, Inorg. Chem.*, 1969, **8**, 170 (*ir*)
Escard, J. *et al, Inorg. Chem.*, 1974, **13**, 695 (*pe*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 281 (*rev, bibl*)

$C_4MnN_4S_4^{2\ominus}$ IC-004528

Tetrakis(thiocyanato-*N*)manganate(*II*)(2−), 11CI

Tetraisothiocyanatomanganate(2−)

$[Mn(NCS)_4]^{2\ominus}$ (T_d)

M 287.2 (ion)

Hg(II) *salt:*
$C_4HgMnN_4S_4$ M 487.8
Synth. from $Mn(SCN)_2$ and $Hg(SCN)_2$ in H_2O. Golden yellow grains, stable to air and H_2O. Mn coordinated to 4 N atoms and Hg to 4 S atoms in approx. tetrahedral geometry with Hg—S—C—N—Mn bridges. Dec. by dil. HCl.

Bis-butyltriphenylammonium salt: Synth. from $MnCl_2.4H_2O$ in EtOH, KSCN in Me_2CO and $[BuPPh_3]SCN$ in EtOH. Pale green cryst. Mp 119°. μ_{eff} = 5.92μ_B (296 K).

Bis-Ph_4As salt: [23303-50-6].
Synth. from $MnCl_2.4H_2O$, KSCN and $[Ph_4As]SCN$ in $EtOH/Me_2CO$. Mp 213°. μ_{eff} = 6.00μ_B (295 K).

Forster, D. *et al, Inorg. Chem.*, 1965, **4**, 715 (*ir*)
Forster, D. *et al, J. Chem. Soc.*, 1965, 268 (*synth, ir, magnetism, struct*)
Scaife, D.E., *Inorg. Chem.*, 1967, **6**, 625 (*synth, struct*)
Salzmann, J.J. *et al, Inorg. Chim. Acta*, 1969, **3**, 207 (*synth, magnetism, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 289; 1981, **C7**, 236 (*rev, bibl*)

$C_4MnN_4Se_4^{2\ominus}$ IC-004529

Tetrakis(selenocyanato-*N*)manganate(*II*)(2−), 9CI

$[Mn(NCSe)_4]^{2\ominus}$ (T_d)

M 474.8 (ion)

Bis-Me_4N salt: Synth. from $Mn(SeCN)_2$ in Me_2CO and $[Me_4N]NCS$ in $MeNO_2$. Pale green. μ_{eff} = 6.07μ_B.

Hexakis(quinoline 1-oxide-O)manganese(2+) salt: [52745-34-3].
$C_{58}H_{42}Mn_2N_{10}O_6Se_4$ M 1400.7
Synth. from $Mn(SeCN)_2$ with quinoline 1-oxide in EtOH. Bright orange cryst.

Foster, D. *et al, Inorg. Chem.*, 1965, **4**, 1712 (*synth, ir, uv, magnetism*)
Salzmann, J.J. *et al, Inorg. Chim. Acta*, 1969, **3**, 207 (*magnetism*)
Schmidtke, H.H. *et al, Z. Naturforsch., A*, 1969, **24**, 126 (*synth, ir*)
Aitken, G.B., *J. Chem. Soc., Dalton Trans.*, 1973, 2637 (*synth, ir, uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 295 (*rev, bibl*)

$C_4MnN_5O^{4\ominus}$ IC-004530

Tetrakis(cyano-*C*)nitrosylmanganate(4−), 10CI

Tetracyanonitrosylmanganate(0)

$[Mn(NO)(CN)_4]^{4\ominus}$

M 189.0 (ion)
Struct. not known.

Tetra-K salt: [63685-31-4].
Synth. from $K_3[Mn(NO)(CN)_5]$ and K in liq. NH_3. Dark green solid.
▷ Ir ν_{NO} 1370 cm^{-1}. Pyrophoric.

Schmidt, J., *Z. Anorg. Allg. Chem.*, 1977, **431**, 284 (*synth, ir*)

$C_4MnO_4^{3\ominus}$ IC-004531

Tetracarbonylmanganate(3−), 10CI

[61769-24-2]

$[Mn(CO)_4]^{3\ominus}$

M 166.9 (ion)

Tri-Na salt: [59123-04-5].
$C_4MnNa_3O_4$ M 235.9
Synth. from $Na[Mn(CO)_5]$ and Na in hexamethylphosphoric triamide. Pale-yellow or light-brown solid. Darkens >320°. Ir ν_{CO} 1792w, 1665vs cm^{-1} (HMPA).

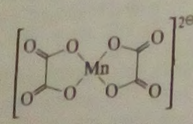
Ellis, J.E. *et al, J. Am. Chem. Soc.*, 1977, **99**, 1801 (*synth, props*)
Organomet. Synth., 1988, **4**, 100 (*synth, ir*)

IC-004532

$C_4MnO_8^{2\ominus}$

Bis(oxalato)manganate(*II*)(2−)
Bis[ethanedioato(2−)-O,O′]manganate(II)(*2−*), *10CI*

[21534-18-9]



M 230.9 (ion)

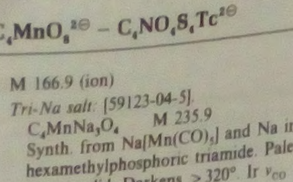
Di-Li salt: [66005-11-6].
Synth. by heating $Mn(OAc)_2$, Li_2CO_3 and oxalic acid. Forms β-Li_2MnO_3 at 600° in O_2.
Di-K salt: Synth. by heating $K_2[Mn(C_2O_4)_2(H_2O)_2]$. See also Diaquabis(oxalato)manganate(*II*)(2−), IC-003934.

Nagase, K. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 868 (*synth, ir, thermal dec*)
Saikali, Y., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1977, **285**, 563 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 104 (*rev, bibl*)

IC-004533

$C_4Mn_2N_8O_4^{4\ominus}$

Tetrakis(cyano-*C*)tetranitrosyldimanganate(4−)
Tetra(cyano-C)tetranitrosyldimanganate(4−)



cis,cis-form

M 333.9 (ion)
Unknown whether two Mn's are staggered or eclipsed.

cis,cis-form

Tetra-K salt: [26998-49-2].
$C_4K_4Mn_2N_8O_4$ M 490.3
Synth. from $Mn(CO)(NO)_3$ and KCN in liq. NH_3. Pale-yellow cryst. Sol. H_2O, EtOH, THF, liq. NH_3. Ir ν_{CN} 2174s, 2125m; ν_{NO} 1737s, 1664vs cm^{-1} (KBr). Diamagnetic.

trans,trans-form

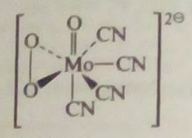
Tetra-K salt: [26658-28-6].
Synth. by heating the *cis*-compd. in EtOH in a sealed tube for several days. Blue-grey needles. Insol. EtOH, sol. liq. NH_3. Ir ν_{CN} 2137s, 2100vs; ν_{NO} 1750s, 1709vs cm^{-1} (KBr).

Behrens, H. *et al, Z. Anorg. Allg. Chem.*, 1969, **365**, 119 (*synth, ir, uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 280 (*rev, bibl*)
Compr. Org. Chem., Pergamon, Oxford, 1982, **4**, 1 (*rev, bibl*)

IC-004534

$C_4MoN_4O_3^{2\ominus}$

Tetrakis(cyano-*C*)oxoperoxymolybdate(*VI*)(2−), 11Cl, 10Cl



M 248.0 (ion)
Pentagonal bipyramidal anion. ^{17}O nmr distinguishes oxo and peroxy ligands.

Bis[bis(triphenylphosphine)iminium] salt: [72969-39-2].
Yellow-amber cryst. Ir ν_{O-O} 900 cm^{-1}.

Arzoumanian, H. *et al, J. Am. Chem. Soc.*, 1980, **102**, 845 (*synth, ir*)
Arzoumanian, H. *et al, J. Mol. Catal.*, 1980, **7**, 43.
Postel, M. *et al, J. Am. Chem. Soc.*, 1983, **105**, 4922 (*O-17 nmr, ir*)

IC-004535

$C_4MoO_4^{4\ominus}$

Tetracarbonylmolybdate(4−)

$[Mo(CO)_4]^{4\ominus}$

M 207.9 (ion)

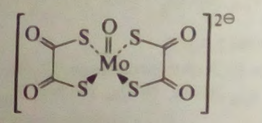
Tetra-Na salt: [67202-63-5].
$C_4MoNa_4O_4$ M 299.9
Used to synth. organometallics. Orange-yellow powder, best used *in situ*. Insol. THF, HMPA, liq. NH_3. Ir ν_{CO} 1680w, 1471s,br cm^{-1} (silicone mull).
▷ Extremely pyrophoric, reacting explosively with fluorolube, water or air. Deflagrates on percussion.

Lin, J.T. *et al, J. Am. Chem. Soc.*, 1983, **105**, 2296 (*synth, ir, haz, use*)

IC-004536

$C_4MoO_5S_4^{2\ominus}$

Bis(1,2-dithiooxalato)oxomolybdate(*IV*)(2−)
Bis[ethanebis(thioato)(2−)-S,S′]oxomolybdate(IV)(*2−*), *10CI*



M 352.2 (ion)
Square pyramidal.

Di-Cs salt: [71147-32-5].
Cryst. + $1H_2O$.

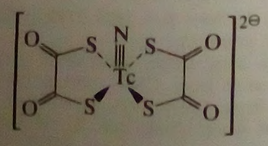
[71214-18-1]

Mennemann, K. *et al, J. Chem. Res. (M)*, 1979, 1372 (*cryst struct, synth, ir*)

IC-004537

$C_4NO_4S_4Tc^{2\ominus}$

Bis(dithiooxalato)nitridotechnetate(*V*)(2−)
Bis[ethanebis(thioato)(2−)-S,S′]nitridotechnetate(V)(*2−*), *12CI*



M 353.2 (ion)

Square-pyramidal anion. Synth. from $TcNCl_4^{\ominus}$ and potassium dithiooxalate. Oxidised and dec. by Cl_2 to give $TcNCl_4^{\ominus}$.

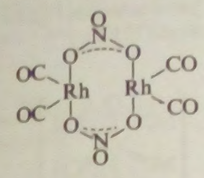
Bis-Ph_4As salt: [117063-57-7].
Pale purple solid. Mp *ca.* 215° dec. Exists in triclinic and monoclinic forms.

Colmanet, S.F. *et al, Inorg. Chim. Acta*, 1988, **147**, 173 (*synth, ir, cryst struct*)
Baldas, J. *et al, J. Nucl. Med.*, 1989, **30**, 1240 (*hplc, biodistrib*)
Abram, U. *et al, Inorg. Chim. Acta*, 1990, **169**, 49 (*synth, uv, esr, cryst struct*)

IC-004538

$C_4N_2O_{10}Rh_2$

Bis(nitrato)tetracarbonyldirhodium
Bis-μ-nitratobis[dicarbonylrhodium]



M 441.8
Moisture-sensitive, purple solid by subl. Mp 100-105° dec. Subl. 80° *in vacuo*. Ir ν_{CO} 2123vs, 2081m, 2037vs, 2000s, 1992m cm^{-1} (nujol).

Lawson, D.N. *et al, J. Chem. Soc.*, 1965, 1900 (*synth, ir*)

IC-004539

$C_4N_4Ni^{4\ominus}$

Tetrakis(cyano-*C*)nickelate(4−), 9CI
Tetracyanonickelate(0)(*4−*)

[59471-59-9]

$[Ni(CN)_4]^{4\ominus}$

M 162.7 (ion)
Assumed tetrahedral struct. Synth. from $[Ni(CN)_4]^{2\ominus}$ + K in NH_3(l). V. reducing; converts H_2O to H_2. Some $CN^{\ominus}$ easily replaced by CO, PR_3 etc.

Tetra-K salt: [15321-21-8].
$C_4K_4N_4Ni$ M 319.1
Yellow solid.

Eastes, J.W. *et al, J. Am. Chem. Soc.*, 1942, **64**, 1187 (*synth*)
de Haas, K.S. *et al, Inorg. Chim. Acta*, 1977, **24**, 269 (*ir, uv*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 6,7.

IC-004540

$C_4N_4Ni^{3\ominus}$

Tetrakis(cyano-*C*)nickelate(3−), 9CI
Tetracyanonickelate(I)(*3−*)

[42985-62-6]

$[Ni(CN)_4]^{3\ominus}$

M 162.7 (ion)
Paramagnetic. Struct. unknown. Prepd. from Tetrakis(cyano-*C*)nickelate(2−), IC-004541 and N_2H_4 in alkali.

Tri-K salt:
$C_4K_3N_4Ni$ M 280.0
Bright red solid.

Nast, R. *et al, Z. Naturforsch., B*, 1954, **9**, 798 (*synth, magnetism*)

IC-004541

$C_4N_4Ni^{2\ominus}$

Tetrakis(cyano-*C*)nickelate(2−), 9CI
[15453-80-2]

$[Ni(CN)_4]^{2\ominus}$ (D_{4h})

M 162.7 (ion)
▷ Toxic. Mutagenic.

Di-Na salt: [14038-85-8].
Catalyst for alkyne hydrogenation, hydrocyanation and hydrogenation-rearrangement of butene. Catalyst for vat dye printing. Transparent yellow-orange hexagonal prisms or needles + $3H_2O$ (H_2O). Sol. H_2O. Dehydrates at 110°.
Di-K salt: [14220-17-8].
Used in indirect complexometric titration determination of silver, and titrimetric determination of phosphorus. Catalyst in polymerisation of vinyl compds. Red-orange cryst. + $1H_2O$ (H_2O). V. sol. H_2O. Monohydrate dehydrates at 100°. Dec. in mineral acid.
▷ QR8650000.

Bis(tetrabutylammonium) salt: [21518-38-7].
Catalyst in ethylene polym.

[14323-41-2, 15453-80-2, 19554-32-6, 48042-08-6]

Inorg. Synth., 1946, **2**, 227 (*synth*)
Larsen, F.K. *et al, Acta Chem. Scand.*, 1967, **23**, 61 (*struct*)
Mason, W.R. *et al, J. Am. Chem. Soc.*, 1968, **90**, 5721 (*uv*)
Jones, D. *et al, Spectrochim. Acta, Part A*, 1968, **24**, 973.
Matienzo, J. *et al, Inorg. Chem.*, 1973, **12**, 2762 (*pe*)
Cowman, C.D. *et al, J. Am. Chem. Soc.*, 1973, **95**, 7873 (*uv*)
Compr. Coord. Chem., 1987, **5**, 67; **6**, 110, 822, 873.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3195.

IC-004542

$C_4N_4Ni^{\ominus}$

Tetrakis(cyano-*C*)nickelate(1−)
Tetracyanonickelate(III)(*1−*), *8CI*

[53557-21-4]

$[Ni(CN)_4]^{\ominus}$

M 162.7 (ion)
Formed by radiolysis of solns. Tetrakis(cyano-*C*) nickelate(2−), IC-004541.

Mulazzini, Q.J. *et al, Int. J. Radiat. Phys. Chem.*, 1974, **6**, 87.
Symons, M.C.R. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1744 (*esr*)

IC-004543

$C_4N_4NiO_4^{2\ominus}$

Tetrakis(cyanato-*N*)nickelate(2−), 9CI
Tetracyanatonickelate(II)(*2−*), *8CI*

[16338-18-4]

$[Ni(NCO)_4]^{2\ominus}$

M 226.7 (ion)
Tetrahedral. Paramagnetic.

Bis-Et_4N salt:
$C_{20}H_{40}N_6NiO_4$ M 487.2
Deep blue solid. Sol. $MeNO_2$, $PhNO_2$, Me_2CO/Et_2O. Mp 219°.
Bis-Ph_4As salt: Blue cryst. Sol. $MeNO_2$, $PhNO_2$. Mp 173-174°.

[17857-25-9]

Forster, D. *et al, J. Chem. Soc.*, 1964, 2790; 1965, 262 (*synth, uv, ir, elec cond, magnetism*)
Fackler, J.P. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 2035 (*synth, ir, uv, elec cond, magnetism*)

IC-004544

$C_4N_4NiS_4^{2\ominus}$

Tetrakis(thiocyanato-*N*)nickelate(2−)

Tetrakis(isothiocyanato)nickelate(II)(2−), 8CI. Tetraisothiocyanatonickelate(II)(2−)

[15488-98-9]

$[Ni(NCS)_4]^{2\ominus}$

M 291.0 (ion)

Forms blue-green tetrahedral and green-yellow octahedral polymeric salts. See also Diaquatetrakis(thiocyanato-*N*)nickelate(2−), IC-003938. Paramagnetic.

Bis-Et_4N salt: Apple-green solid. Mp 284° dec.

Bis-Ph_4As salt: Blue-green and olive-yellow forms. Heating olive-yellow form to ~155° gives blue-green form.

[15955-89-2, 52666-74-7]

Forster, D. *et al, Inorg. Chem.*, 1965, **4**, 715, 823 (*synth, ir*)
Mattenzo, J. *et al, Inorg. Chem.*, 1973, **12**, 2769 (*pe*)

IC-004545

$C_4N_4NiSe_4^{2\ominus}$

Tetrakis(selenocyanato-*N*)nickelate(2−), 12CI

Tetraisoselenocyanatonickelate(II)(2−)

[30908-80-6]

$[Ni(NCSe)_4]^{2\ominus}$

M 478.6 (ion)

Octahedral struct. suggested, with coordination to neighbouring SeCN groups, forming polymeric struct.

[1,4-Phenylenebis(methylene)]bis[triphenylphosphonium](2+) salt:

$C_{68}H_{56}N_4NiP_2Se_4$ M 1107.3

Yellow solid. Ir ν_{CSeN} 2145m, 2092vs, 2075s; ν_{CSe} 653vw; ν_{NiN} 237s cm^{-1} (nujol). Paramagnetic, μ_{eff} = 3.17μ_B (290K).

Bis[methylmercury(1+)] salt: [105832-91-5].

$C_6H_6Hg_2N_4NiSe_4$ M 909.8

Sky blue solid. Mp 186° dec. Ir ν_{CN} 2175s, 2110s; ν_{CSe} 590s, 520s cm^{-1}. Paramagnetic, μ_{eff} = 3.02 μ_B. Forms adducts with Py.

Bis[ethylmercury(1+)] salt: [105832-92-6].

$C_8H_{10}Hg_2N_4NiSe_4$ M 937.9

Sky blue solid. Mp 192° dec. Paramagnetic, μ_{eff} = 2.95μ_B. Ir ν_{CN} 2168s, 2125s; ν_{CSe} 578s, 530sh cm^{-1}. Adduct formed with Py.

Bis[propylmercury(1+)] salt: [105832-93-7].

$C_{10}H_{14}Hg_2N_4NiSe_4$ M 965.9

Sky blue solid. Mp 205° dec. Paramagnetic, μ_{eff} = 2.98μ_B. Ir ν_{CN} 2175, 2118; ν_{CSe} 610s,540s cm^{-1}. Adduct formed with Py.

μ-1,1′-Ferrocenediyldimercury(2+) salt: [115587-19-4].

$C_{14}H_8FeHg_2N_4NiSe_4$ M 1063.8

Light brown cryst. (Me_2CO/EtOH). Mp 154° dec. Paramagnetic, μ_{eff} = 3.01μ_B. Ir ν_{CN} 2165s, 2105sh, 2040s; ν_{CSe} 735s, 520s cm^{-1}. Adducts formed with Py, bipy, phen.

Forster, D. *et al, Inorg. Chem.*, 1965, **4**, 1712 (*synth, ir, esr, magnetism*)
Singh, V.P., *Synth. React. Inorg. Metal-Org. Chem.*, 1985, **15**, 1189 (*synth, derivs, props, ir*)
Singh, P.P. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1987, **17**, 361 (*synth, derivs, props, ir*)

$C_4N_4OS_4V^{2\ominus}$

IC-004546

Oxotetrakis(thiocyanato-*N*)vanadate(*IV*)(2−), 11CI

Tetrakis(isothiocyanato)oxovanadate(IV)(2−), 8CI

[52645-37-1]

$[VO(NCS)_4]^{2\ominus}$

M 299.2 (ion)

Di-K salt: [24947-13-5].
Synth. from KNCS and $VOSO_4$ in aq. soln. Grey-blue solid (H_2O).

Bis-Et_4N salt: [52645-38-2].
Synth. from $VOCl_3$, KSCN and Et_4NCl in MeCN and heating the product to remove MeCN.

[21136-26-5, 34287-47-3]

Kerridge, D.H. *et al, J. Chem. Soc. A*, 1969, 2211 (*synth, K salt*)
Bailey, R.A. *et al, Coord. Chem. Rev.*, 1971, **6**, 407 (*ir*)
Bailey, R.A. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 3206 (*ir*)
Brunette, J.P. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **278**, 347 (*synth, ir, Et_4N salt*)

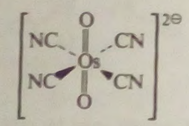
IC-004547

$C_4N_4O_2Os^{2\ominus}$

Tetrakis(cyano-*C*)dioxoosmate(*VI*)(2−)

Tetracyanodioxoosmate(VI)(2−)

[89907-04-0]



M 326.2 (ion)

Synth. by acidification of aq. $[OsO_2(OH)_4]^{2\ominus}$ in the presence of $CN^{\ominus}$, with HOAc. *trans*-Dioxoosmium(*VI*) complexes function as powerful one-electron oxidants.

Di-K salt: [22639-14-1].
Ir ν_{NO_2} 830, 280 cm^{-1}.

Griffith, W.P., *J. Chem. Soc.*, 1964, 245 (*ir*)
Griffith, W.P. *et al, J. Chem. Soc. A*, 1969, 24 (*ir*)
Hanuza, J. *et al, Acta Phys. Pol. A*, 1972, **42**, 537 (*ir*)
Opekar, F. *et al, Electrochim. Acta*, 1977, **22**, 243 (*electrochem*)
Packard, A.B. *et al, Acta Chem. Scand.*, 1984, **241**, 51 (*use*)
Yam, V.W.W. *et al, J. Chem. Soc., Chem. Commun.*, 1988, 100 (*use*)
Preetz, W. *et al, Z. Naturforsch., B*, 1988, **43**, 94 (*synth, ir, raman*)
Yam, V.W.W. *et al, Coord. Chem. Rev.*, 1990, **97**, 93 (*rev*)

IC-004548

$C_4N_4O_2Re^{3\ominus}$

Tetrakis(cyano-*C*)dioxorhenate(*V*)(3−), 11CI

Tetracyanodioxorhenate(V)(3−)

[20756-46-1]

$[ReO_2(CN)_4]^{3\ominus}$

M 322.2 (ion)

Octahedral.

***trans*-form**

Interatomic distances: Re=O 177.3, Re—C 211.5, 213.2 pm.

Tri-K salt: [19439-48-6].
Synth. from K_2ReCl_6, KCN and H_2O_2 or from $ReOCl_2(OEt)(PPh_3)_2$ and KCN in MeOH. Orange cryst. (H_2O).

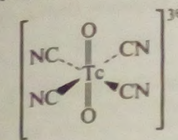
Lock, C.J.L. *et al, J. Chem. Soc.*, 1964, 2281 (*synth, ir, props*)
Beard, J.H. *et al, J. Am. Chem. Soc.*, 1968, **90**, 3389 (*synth*)
Murmann, R.K. *et al, Inorg. Chem.*, 1971, **10**, 2352 (*synth*)
Fenn, R.H. *et al, J. Chem. Soc. A*, 1971, 2880 (*cryst struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Academic Press, N.Y., 1975-1981, **3**, 1631 (*synth*)
Winkler, J.R. *et al, Inorg. Chem.*, 1985, **24**, 346 (*synth, uv*)

IC-004549

$C_4N_4O_2Tc^{3\ominus}$

Tetrakis(cyano-*C*)dioxotechnetate(*V*)(3−), 10CI

Tetracyanodioxotechnetate(V)(3−)



M 234.9 (ion)

trans-Octahedral anion. Synth. by hydrol. of $[TcO(CN)_5]^{2\ominus}$, or by reaction of $[TcO_2Py]^{\ominus}$ with aq. KCN.

Tri-K salt: [73466-61-2].
Lemon yellow needles (MeOH aq.).

Trop, H.S. *et al, Inorg. Chem.*, 1980, **19**, 1993 (*synth, uv, ir*)

IC-004550

$C_4N_4O_4Pt^{2\ominus}$

Tetrakis(isocyanato-*N*)platinate(2−), 8CI

Tetracyanatoplatinate(II)

$[Pt(NCO)_4]^{2\ominus}$

M 363.1 (ion)

Square planar. Ligand binds through N atom.

Bis-Et_4N salt: [21283-66-9].
Off white solid. Sol. Me_2CO, $MeNO_2$.

Bis-Ph_4As salt: [21283-65-8].
Off white solid. Sol. CH_2Cl_2, $MeNO_2$.

[88358-83-2]

Norbury, A.H. *et al, J. Chem. Soc. A*, 1968, 1598.

IC-004551

$C_4N_4O_4Si$

Silicon tetraisocyanate

Tetraisocyanatosilane, 9CI. Tetrakis(isocyanato)silane. Silicon(IV) isocyanate

[3410-77-3]

$Si(NCO)_4$

M 196.1

Efficient reagent for synth. of ureas from amines. Insol. Me_2CO; sol. C_6H_6, CCl_4, CS_2; dec. in H_2O. d_4^{25} 1.434. Mp 26°. Bp 185-186°.

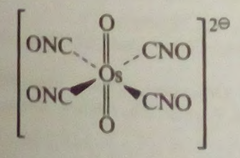
Miller, F.A., *Spectrochim. Acta*, 1961, **17**, 977 (*ir, struct*)
Inorg. Synth., 1966, **8**, 23; 1986, **24**, 99 (*synth*)
Hjortaas, K.E., *Acta Chem. Scand.*, 1967, **21**, 1381 (*struct*)
Miller, F.A., *Appl. Spectrosc.*, 1975, **29**, 461 (*spectra*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 704 (*synth*)
Graddon, D.P. *et al, J. Organomet. Chem.*, 1978, **148**, 17.
Barta, I.A. *et al, J. Organomet. Chem.*, 1980, **185**, 323 (*ir, struct*)

IC-004552

$C_4N_4O_6Os^{2\ominus}$

Tetrakis(fulminato)dioxoosmate(*VI*)(2−)

[45151-86-8]



M 390.2 (ion)

trans-Octahedral.

Bis-Ph_4As salt: [30870-31-6].

Synth. from OsO_4, $Hg(CNO)_2$ and amalgamated K followed by pptn. with $[AsPh_4]Cl$. Brown solid. Mp 121°. Ir ν_{CN} 2297, 2181; ν_{CNO} 1147; ν_{OsO_2} 824 cm^{-1}.

Beck, W. *et al, Chem. Ber.*, 1970, **103**, 3591 (*synth, ir*)

IC-004553

$C_4N_4OsS_4^{2\ominus}$

Tetrakis(thiocyanato)osmate(*II*)(2−)

$[Os(SCN)_4]^{2\ominus}$

M 422.5 (ion)

Pilipenko, A.T. *et al, Ukr. Khim. Zh. (Russ. Ed.)*, 1968, **34**, 755; 1970, **36**, 1257 (*ir*)
Pilipenko, A.T. *et al, Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1970, 87.

IC-004554

$C_4N_4P_2$

Hypodiphosphorous tetracyanide, 10CI

Tetracyanodiphosphine. Tetracyanodiphosphorus(III)

[4638-31-7]

$(NC)_2PP(CN)_2$

M 166.0

Synth. from P_2I_4 + AgCN. Unstable liq., v. sensitive to oxidation and hydrol. Disproportionates and polymerises.

Baudler, M. *et al, Z. Naturforsch., B*, 1965, **20**, 494 (*synth, ir, props*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, London, 1971, **8/III**, 584 (*rev, bibl*)
Dillon, K.B. *et al, Inorg. Nucl. Chem. Lett.*, 1981, **17**, 201 (*synth, P-31 nmr*)
Grobe, J. *et al, Z. Anorg. Allg. Chem.*, 1985, **526**, 145 (*synth, ir, ms, P-31 nmr, complexes*)

IC-004555

$C_4N_4Pd^{2\ominus}$

Tetrakis(cyano-*C*)palladate(2−), 9CI

Tetracyanopalladate(II)

[15004-87-2]

$[Pd(CN)_4]^{2\ominus}$

M 210.4 (ion)

Di-K salt: [14516-46-2].
Prepd. by dissolving $Pd(CN)_2$ in aq. KCN. White cryst. + $3H_2O$ (H_2O). Heating to 100° gives the monohydrate. V. sol. H_2O; mod. sol. EtOH.

Inorg. Synth., 1946, **2**, 245 (*synth*)
Jerome-Lerutte, S., *Struct. Bonding (Berlin)*, 1972, **10**, 153 (*ir, struct, rev*)
Moreau-Colin, M.L., *Struct. Bonding (Berlin)*, 1972, **10**, 167 (*uv, struct, rev*)
Sano, M. *et al, Inorg. Chem.*, 1982, **21**, 2521 (*cmr, N-15 nmr*)

IC-004556

$C_4N_4PdS_4^{2\ominus}$

Tetrakis(thiocyanato-*S*)palladate(2−), 9CI

Tetrathiocyanatopalladate(II)

[16057-01-5]

$[Pd(SCN)_4]^{2\ominus}$

M 338.7 (ion)

Di-K salt: [14516-47-3].
Prepd. by adding aq. KSCN to aq. K_2PdCl_4. Dark brownish-red needles.

[37234-71-2]

Sabatini, A. *et al, Inorg. Chem.*, 1965, **4**, 959 (*ir*)

Mawby, A. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 2213 (*cryst struct*)
De Strefano, N.J. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1973, **3**, 313 (*synth*)
Kargol, J.A. *et al, Inorg. Chem.*, 1979, **18**, 2532 (*cmr*)

IC-004557

$C_4N_4PdSe_4^{2\ominus}$

Tetrakis(selenocyanato-*Se*)palladate(*II*)(2−)
Tetraselenocyanatopalladate(II)

$[Pd(SeCN)_4]^{2\ominus}$

M 526.3 (ion)
Bis-Me_4N salt: Brown solid (EtOH). Mp 120°. Ir ν_{CN} 2114, 2105 cm^{-1} (nujol).
Bis-Et_4N salt: [15663-58-8].
Red brown cryst. Mp 102-103°. Ir ν_{CN} 2116 cm^{-1} (KBr).
Bis-tetrabutylammonium salt: [15639-12-0].
Red brown solid. Ir ν_{CN} 2107 cm^{-1} (nujol), 2113 cm^{-1} (Me_2CO).

Forster, D. *et al, Inorg. Chem.*, 1965, **4**, 1712 (*synth, ir*)
Burmeister, J.L. *et al, Inorg. Chem.*, 1966, **5**, 1113 (*synth, ir, uv-vis*)
Schmidtke, H.-H. *et al, Helv. Chim. Acta*, 1967, **50**, 1631 (*synth, ir, uv-vis*)
Kargol, J.A. *et al, Inorg. Chem.*, 1979, **18**, 2532 (*cmr*)

IC-004558

$C_4N_4Pt^{2\ominus}$

Tetrakis(cyano-*C*)platinate(2−), 9CI
Tetracyanoplatinate(II)(2−)
[15004-88-3]

$[Pt(CN)_4]^{2\ominus}$

M 299.1 (ion)
Classic square planar complex. V. many salts known; colours varying with cations and degree of hydration. Properties v. much studied, particularly structs. and physical properties of salts with Pt cations and partially oxidised materials.
Di-K salt: [562-76-5].
$C_4K_2N_4Pt$ M 377.3
V. stable. Yellow-green needles + $3H_2O$. Yellow product can form; which is possibly the monohydrate. Several hydrates known.
Di-Cs salt: [15747-35-0].
$C_4Cs_2N_4Pt$ M 564.9
Blue-white cryst. + H_2O. Several hydrates known.
Ba salt: [562-81-2].
C_4BaN_4Pt M 436.4
Useful in synth. of partially oxidised $Pt(CN)_4^{2\ominus}$ salts. Has been used in fluorescent X ray screens. Yellow-green or colourless cryst. + $4H_2O$.
▷ Hazardous synth.

Tetracyanoplatinate(1.75−)
Part. oxidised-form
Representative formula for range of compds. with important chain structs. leading to 1-D electrical conductance. Other examples contain anions, eg. $K_2[Pt(CN)_4]Br_{0.3}.3.2H_2O$, sometimes known as Krogmann salts.
K salt (1:1.75):
$C_4K_{1.75}N_4Pt$ M 367.5
Bronze-coloured cryst. + 1.5 H_2O (H_2O). Loses H_2O easily.
Cs salt (1:1.75):
$C_4Cs_{1.75}N_4Pt$ M 531.7
Copper-brown needles + $2H_2O$. Loses H_2O easily.

[13755-32-3, 14323-36-5, 16457-34-4, 38245-27-1, 59831-03-7, 83018-11-5, 87826-97-3]

Gmelin Handbook Inorg. Chem., Syst. No. 68, 1939, **C**, 125, 142, 163, 204 (*rev, bibl*)
Inorg. Synth., 1979, **19**, 3, 6, 8, 13, 112 (*synths, partially oxid deriv*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 375.

IC-004559

$C_4N_4PtS_4^{2\ominus}$

Tetrakis(thiocyanato-*S*)platinate(2−)
Tetrathiocyanatoplatinate(II)
[38668-99-4]

$[Pt(SCN)_4]^{2\ominus}$

M 427.4 (ion)
Ligand binds through S atoms, but linkage isomers found in CH_2Cl_2 soln. of $Bu_4N^{\oplus}$ salt.
Di-K salt: [14244-61-2].
$C_4K_2N_4PtS_4$ M 505.6
Red solid. Sol. H_2O.
▷ TP1870000.
Bis-tetrabutylammonium salt: [73297-67-3].
Red solid. Sol. polar org. solvs.

[17731-25-8]

de Strefano, N.J. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1973, **3**, 313 (*synth*)
Norbury, A.H., *Adv. Inorg. Chem. Radiochem.*, 1975, **17**, 231 (*rev*)
Kargol, J.A. *et al, Inorg. Chem.*, 1979, **18**, 2532 (*cmr*)
Tusznski, W. *et al, Z. Naturforsch., A*, 1979, **34**, 211 (*uv-vis*)
Pregosin, P.S. *et al, Inorg. Chim. Acta*, 1980, **38**, 237 (*N-15 nmr, Pt-195 nmr*)

IC-004560

$C_4N_4PtSe_4^{2\ominus}$

Tetrakis(selenocyanato-*Se*)platinate(2−)
Tetraselenocyanatoplatinate(II), *8CI*

$[Pt(SeCN)_4]^{2\ominus}$

M 614.9 (ion)
Ligand binds through Se known as $R_4N^{\oplus}$ salts.
Bis-Et_4N salt: [15624-47-2].
Red cryst. Sol. polar org. solvs.
Bis-tetrabutylammonium salt: Reddish brown solid. Sol. polar org. solvs.

Burmeister, J.L. *et al, Inorg. Chem.*, 1966, **5**, 1113 (*synth, ir, elec cond*)
Schmidtke, H.H. *et al, Helv. Chim. Acta*, 1967, **50**, 1631 (*synth, ir, elec cond*)

IC-004561

$C_4N_4S_4Si$

Silicon tetraisothiocyanate
Tetraisothiocyanatosilane, 9CI. Tetrakis(isothiocyanato) silane. Tetrakis(thiocyanato-N)silicon
[6544-02-1]

$Si(NCS)_4$ (T_d)

M 260.4
Reacts with amines to generate thioureas. Mp 143.8°, Mp 143-144°. Bp 313°, Bp 314°.

Inorg. Synth., 1966, **8**, 27 (*synth*)
Tames, N. *et al, Acta Chim. Acad. Sci. Hung.*, 1978, **96**, 217 (*synth, uv*)
Barta, I.A. *et al, J. Organomet. Chem.*, 1980, **185**, 323 (*ir, struct*)
Kolodyazhniya, Yu.V. *et al, Zh. Obshch. Khim.*, 1983, **53**, 2266

IC-004562

$C_4N_4S_4Th$

Thorium(*IV*) thiocyanate
Tetrakis(thiocyanato)thorium(IV)
[21563-88-2]

$Th(NCS)_4$

M 464.3
Identified in thermal dec. of various complexes. Isol. of anhyd. compd. not confirmed. Obt. as tetrahydrate. Reported to dec. in air to $ThO(NCS)_2$ > 280°.
Tetrahydrate:
$C_4H_8N_4O_4S_4Th$ M 536.4
V. hygroscopic white solid. V. sol. H_2O; sol. EtOH, MeOH, Me_2CO. Photosensitive.

Molodkin, A.K. *et al, Zh. Neorg. Khim.*, 1964, **9**, 60; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 32 (*synth*)
Agarwal, R.K. *et al, J. Inorg. Nucl. Chem.*, 1980, **42**, 1366; 1981, **43**, 203.
Agarwal, R.K. *et al, Transition Met. Chem.*, 1980, **5**, 237.
Agarwal, R.K. *et al, Thermochim. Acta*, 1982, **56**, 247 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 44, *Suppl. Vol.*, 1988, C7, 18 (*rev*)

IC-004563

$C_4N_4S_4U$

Uranium(*IV*) thiocyanate
Uranium tetrakis(thiocyanate)

$U(NCS)_4$

M 470.3
Has never been isol. as a solid. Stabilised as complex $U(NCS)_4(OH_2)_4$ molecules in crown-ether complex.
18-Crown-6 complex (1:1.5):
$C_{22}H_{36}N_4O_9S_4U$ M 866.8
Deep green cryst. 8-Coord. square antiprismatic at U.

Charpin, P. *et al, Inorg. Nucl. Chem. Lett.*, 1977, **13**, 341 (*synth, ir, uv, cryst struct*)

IC-004564

$C_4N_4Ti^{4\ominus}$

Tetrakis(cyano-*C*)titanate(4−), 10CI
Tetracyanotitanate(0)

$[Ti(CN)_4]^{4\ominus}$

M 151.9 (ion)
Tetra-K salt: [54836-64-5].
$C_4K_4N_4Ti$ M 308.3
Synth. by reducing mixt. of $TiBr_3$ and KCN with K in liq. NH_3. Black solid; readily oxidised and hydrol. Paramagnetic, $\mu_{eff} = 2.17\mu_B$, g = 1.993.
▷ Pyrophoric in air. Cyanides are toxic.

Nicholls, D. *et al, Inorg. Chim. Acta*, 1980, **41**, 233 (*synth, ir, uv-vis, magnetism*)

IC-004565

$C_4N_4Ti^{2\ominus}$

Tetrakis(cyano-*C*)titanate(2−), 10CI
Tetracyanotitanate(II)

$[Ti(CN)_4]^{2\ominus}$

M 151.9 (ion)
Octahedral polymer.
Di-K salt: [75038-71-0].
$C_4K_2N_4Ti$ M 230.1
Synth. by reduction of $K_3Ti(CN)_6$ with K in liq. NH_3. Black solid. Readily hydrol. in aq. NH_3 yielding $Ti(OH)_2$, then $Ti(OH)_3$. Paramagnetic, $\mu_{eff} = 1.19\mu_B$.

Nicholls, D. *et al, Inorg. Chim. Acta*, 1980, **41**, 233 (*synth, ir, uv-vis, magnetism*)

IC-004566

C_4N_4Ti

Titanium(*IV*) cyanide ($Ti(CN)_4$), 10CI
Tetracyanotitanium(IV). *Titanium tetracyanide. Tetrakis(cyano-C)titanium*
[67847-25-0]

$Ti(CN)_4$

M 151.9
Synth. analogous to Zirconium(*IV*) cyanide ($Zr(CN)_4$), IC-004569. Brown solid. Insol. common org. solvs.

Gorsi, B.L. *et al, J. Indian Chem. Soc.*, 1978, **55**, 321 (*synth, ir*)

IC-004567

$C_4N_4V^{2\ominus}$

Tetrakis(cyano-*C*)vanadate(*II*)(2−), 11CI
Tetracyanovanadate(II)(2−)

$[V(CN)_4]^{2\ominus}$

M 155.0 (ion)
Di-K salt: [82728-69-6]. *Potassium tetracyanovanadate*(II) ($K_2V(CN)_4$)
$C_4K_2N_4V$ M 233.2
Synth. by oxidising K salt of Bis(cyano-*C*) vanadate(2−), IC-003487 with NH_4CN in liq. NH_3. Pale purple solid. Paramagnetic; $\mu_{eff} = 3.2\mu_B$.
▷ Toxic.

Dodsworth, E.S. *et al, Inorg. Chim. Acta*, 1982, **61**, 9 (*synth, magnetism, ir, uv-vis*)

IC-004568

$C_4N_4Zr^{2\ominus}$

Tetrakis(cyano-*C*)zirconate(*II*)(2−), 11CI
Tetracyanozirconate(II)

$[Zr(CN)_4]^{2\ominus}$

M 195.2 (ion)
Di-K salt: [93293-91-5].
$C_4K_2N_4Zr$ M 273.4
Synth. from $K_2Zr(CN)_6$ and NH_4CN in liq. NH_3. Mauve solid. Paramagnetic, $\mu_{eff} = 2.75\mu_B$ (293K).
▷ Cyanides are toxic.

Dodsworth, E.S. *et al, Inorg. Chim. Acta*, 1984, **89**, 143 (*synth, ir, uv/vis, magnetism*)

IC-004569

C_4N_4Zr

Zirconium(*IV*) cyanide ($Zr(CN)_4$), 10CI
Tetracyanozirconium(IV). *Zirconium tetracyanide. Tetrakis(cyano-C)zirconium*
[67847-26-1]

$Zr(CN)_4$

M 195.2
Synth. by reaction of $Zr[OCH(CH_3)_2]_4$ with 4 H_3CCOCN. Blackish-brown solid. Sol. Me_2CO.
$Zr[OCH(CH_3)_2]_n(CN)_{4-n}$ ($n = 1 - 4$) can be isol. by changing the ratio of reactants.
Diammine complex: [97396-33-3]. *Diamminetetrakis(cyano-C)zirconium, 11CI*
$C_4H_6N_6Zr$ M 229.3
Synth. from $ZrBr_4.2NH_3$ + NH_4CN in liq. NH_3.

Gorsi, B.L. *et al*, *J. Indian Chem. Soc.*, 1978, **55**, 321 (*synth, ir*)
Boyle, E.L. *et al*, *Inorg. Chim. Acta*, 1985, **100**, 281 (*synth, diammine complex*)

IC-004570

$C_4N_5Re^{2\ominus}$

Nitridotetracyanorhenate(V)(2−)

Tetraisocyanonitridorhenate(V)(2−), 8CI

$[NRe(CN)_4]^{2\ominus}$

M 304.2 (ion)

Di-K salt: $C_4K_2N_5Re$ M 382.4
Synth. from $ReNCl_2(PPh_3)_2$ and KCN. Yellow solid + $1H_2O$. Precipitated from aq. soln. by MeOH as salmon-pink cryst.

Johnson, N.P., *J. Chem. Soc. A*, 1969, 1843 (*synth, ir, uv*)
Davies, W.O. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 736 (*cryst struct*)

IC-004571

$C_4N_5S_4Tc^{2\ominus}$

Nitridotetrakis(thiocyanato-*N*)technetate(2−), 11CI

Tetraisothiocyanatonitridotechnetate(V)(2−)

$[TcN(NCS)_4]^{2\ominus}$

M 345.2 (ion)
Thiocyanate N-bonded by implication. Synth. from $TcNCl_4^{\ominus}$ and KNCS.

Bis-tetrabutylammonium salt: [108089-79-8].
Orange brown solid. Mp 114-116°.

Bis-Ph_4As salt: [103948-33-0].
Orange-red solid. Mp 81-85°.

Abram, U. *et al*, *Z. Chem.*, 1986, **26**, 140 (*synth, ir, uv*)
Abram, U. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **544**, 167 (*synth, esr*)

IC-004572

$C_4N_{10}Pt^{2\ominus}$

Diazidotetrakis(cyano-*C*)platinate(2−), 10CI

Diazidotetracyanoplatinate(IV)

As Dibromotetrakis(cyano)platinate(2−), IC-003817 with

$X = N_3$

M 383.1 (ion)
trans-Structure.

▷ Azides are potentially explosive.

***trans*-form** [66901-76-6]
Irradiation of solns. gives N_2 and $[Pt(CN)_4]^{2\ominus}$, but solns. in EtOH may produce rare N_3 radicals.

Di-K salt: Orange cryst. Sol. H_2O, polar org. solvs.

Volger, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1978, **17**, 524 (*ir, uv-vis*)
Weber, W. *et al*, *Inorg. Chim. Acta*, 1986, **111**, 129 (*synth*)

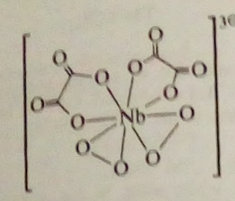
$C_4NbO_{12}^{3\ominus}$

IC-004573

Bis(oxalato)bis(peroxo)niobate(V)(3−)

Bis[ethanedioate(2−)-O,O']diperoxyniobate(V)(3−), 10CI

[55992-16-0]



M 332.9 (ion)
Dodecahedral.

Tris-NH_4 salt: [80004-95-1].
Synth. from oxalic acid and $(NH_4)_3Nb(O_2)_4$ in H_2O.
Yellowish-green solid.

Tris-NH_4 salt, monohydrate: [23388-20-7].
Cryst. (H_2O).

Mathern, G. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 1572 (*synth, cryst struct*)
Shchelokov, R.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1972, **17**, 2433 (*synth, ir*)

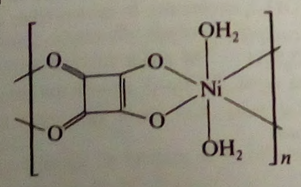
IC-004574

C_4NiO_4

Nickel(II) squarate

[3,4-Dihydroxy-3-cyclobutene-1,2-dionato(2−)-O^3,O^4]nickel(II), 11CI. (Dihydroxycyclobutenedionato)nickel, 8CI

[33684-90-1]



dihydrate

M 170.7

Dihydrate: Diaqua[3,4-dihydroxy-3-cyclobutene-1,2-dionato(2−)-O^3,O^4]nickel(II)
$C_4H_4NiO_6$ M 206.7
Green powder. Nickel ion bound to two H_2O and chelated to two squarate ions. Proposed struct. is a chain polymer.

West, R. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 2589 (*synth, ir*)
Ludi, A. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1968, **7**, 638 (*struct*)
Bailey, R.A. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 2387 (*dec*)

IC-004575

C_4NiO_4

Tetracarbonylnickel(0)

Nickel carbonyl, 9CI. Nickel tetracarbonyl

[13463-39-3]

$Ni(CO)_4$

M 170.7
Catalyst for carbonylations, organic halide couplings, polymerisations and oligomerisations of alkenes and alkynes. Intermed. in Mond process for purifn. of Ni. Colourless, volatile liq., oxidises in air. Sol. EtOH, C_6H_6, $CHCl_3$, Me_2CO, CCl_4. d_4^{20} 1.31. Mp −25°, Mp −17.2°. Bp_{769} 43° (extrap.). Dec. >35°.

▷ Extremely toxic vapour. May ignite in air. Carcinogenic. Causes dermatitis. TLV 0.35. QR6300000.

Dewar, J. *et al*, *J. Chem. Soc.*, 1904, **85**, 203.

Manchot, W. *et al*, *Ber.*, 1929, **62**, 678 (*synth*)
Inorg. Synth., 1946, **2**, 234 (*synth*)
Bodner, G. *et al*, *Inorg. Chem.*, 1975, **14**, 1932 (*cmr*)
Prasad, P.L. *et al*, *J. Chem. Phys.*, 1977, **67**, 4584 (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 250.
Compr. Organomet. Chem., Pergamon, Oxford, 1982, **6/3**, 156; **8**, 777 (*rev, use, catalysis*)
Rösch, N. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 4238 (*props*)
Boix, F. *et al*, *Synth. Commun.*, 1987, **17**, 1149 (*synth*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 519.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 495.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2479.

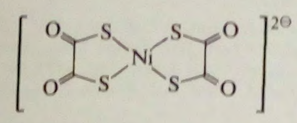
$C_4NiO_4S_4^{2\ominus}$

IC-004576

Bis(dithiooxalato)nickelate(II)(2−), 8CI

Bis[ethanebis(thioato)-S,S']nickelate(II)(2−), 11CI, 9CI

[18443-71-5]



M 298.9 (ion)
Square planar struct. *O* atoms also bond to other metal atoms, e.g. Pd.

red-form
Major form. Useful starting material for range of bimetallic $(C_2S_2O_2)_2$ complexes.

Di-K salt: [25360-81-0].
$C_4K_2NiO_4S_4$ M 377.1
Dark red cryst. (hot H_2O). Sol. hot H_2O, spar. sol. cold H_2O. Early work on dimorphism reports needles when soln. is rapidly cooled to 10° and octahedra if cooled only to 22°. Transition temp. 20°.

black-form
K salt: Formed from red form on heating in dilute $K_2Cr_2O_7$ soln. Glittering black cryst. Struct. comprises stacked anions and linear chains of K.

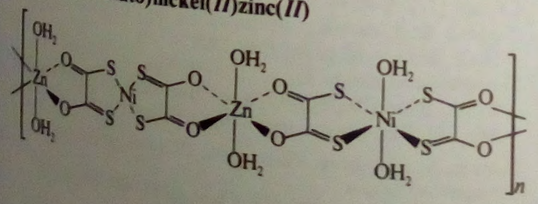
[43030-52-0, 49871-88-7]

Robinson, C.S. *et al*, *J. Chem. Soc.*, 1912, **101**, 62 (*synth, red form, props*)
Latham, A.R. *et al*, *Inorg. Chem.*, 1965, **4**, 788 (*uv*)
Morrison, J.T. *et al*, *Inorg. Chim. Acta*, 1969, **3**, 463 (*synth, uv*)
Coucouvanis, D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 3875 (*cryst struct, red form*)
Gleizes, A. *et al*, *Inorg. Chim. Acta*, 1979, **37**, 19 (*synth, black form, cryst struct*)
Czernuszewicz, R.S. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 1515 (*ir, raman*)
Trombe, J.C. *et al*, *C.R. Hebd. Seances Acad. Sci., Ser. 2*, 1985, **301**, 483 (*lanthanide salts*)

$C_4NiO_4S_4Zn$

IC-004577

Bis(dithiooxalato)nickel(II)zinc(II)



M 364.3 *Hydrate*

Hydrate consists of infinite parallel straight chains of Zn and 4% of the Ni atoms octahedrally coordinated, the rest of the Ni atoms have sq. planar coordination. Thus the system is weakly paramagnetic and non-stoichiometric.

2.08 Hydrate: Synth. from $Zn(ClO_4)_2.6H_2O$ and $K_2Ni(S_2C_2O_2)_2$. Shining black cryst. $\mu_{eff} = 1.02\mu_B$.

Maury, F. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1980, **291**, 49 (*synth, cryst struct, deriv*)

C_4NiS_4

IC-004578

Tetrakis(thiocarbonyl)nickel

Tetrakis(carbonothioyl)nickel, 9CI. Nickel thiocarbonyl

[51062-92-1]

$Ni(CS)_4$ (T_d)

M 234.9
Characterised spectroscopically.

Yarbrough, L.W., *J. Chem. Soc., Chem. Commun.*, 1973, 705 (*ms, ir*)

C_4O

IC-004579

Carbon oxide (C_4O)

4-Oxo-1,2,3-butatriene-1-ylidene, 12CI. Tetracarbon monoxide

[112022-61-4]

$:C{=}C{=}C{=}C{=}O$

M 64.0
Triplet ground state. Formed by the vaporisation of graphite (laser heating) in CO/Ne. Known only in a Ne or Ar matrix.

Van Zee, R.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 609 (*matrix isol, esr*)

C_4O_2

IC-004580

Carbon oxide (C_4O_2)

1,2,3-Butatriene-1,4-dione, 12CI. Tetracarbon dioxide

[51799-35-0]

$O{=}C{=}C{=}C{=}C{=}O$

M 80.0
Prob. has triplet ground state. Formed by flash pyrolysis of cyclic diazoketones with matrix isol. Stable in matrix. Dec. by hv to C_3O and CO.

Maier, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1990, **29**, 905 (*synth, ir, struct*)

$C_4O_4Os^{2\ominus}$

IC-004581

Tetracarbonylosmate(2−), 9CI

$[Os(CO)_4]^{2\ominus}$

M 302.2 (ion)
Usually generated and used *in situ*.

Di-Na salt: [27857-55-2].
$C_4Na_2O_4Os$ M 348.2
Air-sensitive cream-coloured cryst.

Collman, J.P. *et al*, *Inorg. Chem.*, 1974, **13**, 1 (*synth*)
Clark, W.J. *et al*, *Inorg. Chem.*, 1982, **21**, 3955 (*synth*)

C_4O_4Pd IC-004582

Tetracarbonylpalladium

Palladium carbonyl. 9CI. Palladium tetracarbonyl

[36344-80-6]

$Pd(CO)_4$

M 218.4

No physical data available, obt. by matrix isoln.

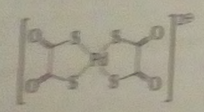
Darling, J.H. *et al. J. Chem. Soc., Dalton Trans.*, 1973, 1879 (synth, ir)

$C_4O_4PdS_2^{2\ominus}$ IC-004583

Bis(dithiooxalato)palladate(*II*)(2−)

Bis[ethanedithioato(2−)-S,S']palladate(2−)

[37378-58-8]



M 346.7 (ion)

Square planar.

Di-K salt: [60490-61-1].

Yellow trigonoidal cryst.

Bis-tetrabutylammonium salt: Yellow cryst. (aq. EtOH). Diamagnetic.

Bis-benzyltriphenylphosphonium salt: [50308-14-0].

Yellow cryst. Sol. $MeNO_2$, DMF. Mp 243-244°. Isomorphous with Ni analogue.

Fujita, J. *et al. Bull. Chem. Soc. Jpn.*, 1964, **37**, 520 (ir)
Latham, A.R. *et al. Inorg. Chem.*, 1965, **4**, 788 (*cis*-cis)
Cox, E.G. *et al. J. Chem. Soc.*, 1935, 1475 (*synth, cryst struct*)
Cotton, F.A. *et al. J. Am. Chem. Soc.*, 1973, **95**, 3775 (*synth, ir*)

C_4O_4Pt IC-004584

Tetracarbonylplatinum

Platinum tetracarbonyl. Platinum carbonyl ($Pt(CO)_4$)

[36344-81-7]

$Pt(CO)_4$ (T_d)

M 307.1

Obt. only by matrix isolation techniques. Dec. below c.t.

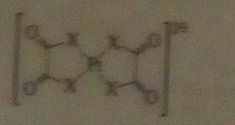
Kündig, E.P. *et al. J. Am. Chem. Soc.*, 1973, **95**, 7234 (ir, raman)
Dixon, A.J. *et al. J. Chem. Soc., Dalton Trans.*, 1988, 1501 (*synth*)

$C_4O_4PtS_2^{2\ominus}$ IC-004585

Bis(dithiooxalato)platinate(*II*), 8CI

Bis[ethanedithioato]platinate(2−), 9CI

[20985-58-6]



X = S

M 435.3 (ion)

Square planar struct.

Di-K salt: [60490-62-2].

Dark red cryst. Sol. H_2O.

$Me^{2\oplus}$ salt: [69958-83-8].

$C_6MeO_4PtS_2$ M 490.3

Black ribbon-shaped cryst. + $7H_2O$.

[46145-21-5]

Cox, E.G. *et al. J. Chem. Soc.*, 1935, 1475 (*synth, cryst struct*)
Fujita, J. *et al. Bull. Chem. Soc. Jpn.*, 1964, **37**, 528 (*ir*)
Latham, A.R. *et al. Inorg. Chem.*, 1965, **4**, 788 (*sac-oxo*)
Gleizes, A. *et al. J. Am. Chem. Soc.*, 1984, **106**, 3727 (*synth, cryst struct*)

$C_4O_4Ru^{2\ominus}$ IC-004586

Tetracarbonylruthenate(2−), 9CI

$[Ru(CO)_4]^{2\ominus}$ (T_d)

M 213.1 (ion)

Di-Na salt: [57398-60-4].

$C_4Na_2O_4Ru$ M 259.0

Synth. by reducing $Ru_3(CO)_{12}$ in liq. NH_3 at −33° with Na metal. A versatile synthetic reagent, particularly for cluster synthesis. Reduces CO_2 to CO. Pale fawn, extremely air-sensitive solid. Sol. polar solvs. (MeOH, THF). Ir ν_{CO} 1940, 1898 cm^{-1} (THF); ν_{CO} 1930, 1887 cm^{-1} (MeOH).

Cotton, J.D. *et al. J. Chem. Soc. A*, 1968, 2162 (*synth, ir*)
Green, M. *et al. J. Chem. Soc., Dalton Trans.*, 1975, 939 (*use*)
Geoffroy, G.L. *et al. J. Am. Chem. Soc.*, 1977, **99**, 7565 (*reactions*)
Benson, I.B. *et al. J. Chem. Soc., Dalton Trans.*, 1978, 1240 (*reactions*)
Muhler, J.M. *et al. J. Am. Chem. Soc.*, 1980, **102**, 7604 (*reduction of CO_2*)

$C_4O_4W^{4\ominus}$ IC-004587

Tetracarbonyltungstate(4−)

$[W(CO)_4]^{4\ominus}$

M 295.8 (ion)

Tetra-Na salt: [67202-46-4].

$C_4Na_4O_4W$ M 387.8

Used in synth. of organometallics. Pale-orange solid, best used *in situ*. Ir ν_{CO} 1679w, 1529s, 1478s,br cm^{-1} (silicone mull).

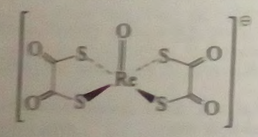
▷ Extremely pyrophoric, reacts explosively with fluorolube; may deflagrate.

Lin, J.T. *et al. J. Am. Chem. Soc.*, 1983, **105**, 2296 (*synth, ir, lsc, use*)

$C_4O_7ReS_4^{\ominus}$ IC-004588

Bis(1,2-dithiooxalato)oxorhenate(*V*)(1−)

Bis[ethanedithioato](2−)-S,S']oxorhenate(V)(1−), 10CI



M 442.5 (ion)

Square pyramidal. Re—S(mean) 233, Re=O 167.4 pm.

Cs salt: [77298-90-9].

Synth. from caesium dithiooxalate and $Cs_2[ReOCl_5]$ in H_2O. Brown-red cryst. (Me_2CO).

Tetrabutylammonium salt: [73396-07-3].

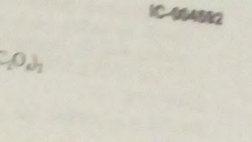
Synth. from $[Bu_4N][ReO_4]$ and potassium dithiooxalate in Me_2CO. Red-brown cryst. (Me_2CO aq.).

Davison, A. *et al. Inorg. Chem.*, 1980, **19**, 1988 (*synth, ir, uv, magnetism, props*)
Matias, R. *et al. Z. Anorg. Allg. Chem.*, 1981, **474**, 216 (*synth, cryst struct, ir*)

$C_4O_8S_4Tc^{\ominus}$ IC-004589

Bis(dithiooxalato)oxotechnetate(*V*)(1−)

Bis[ethanedithioato](2−)-S,S']oxotechnetate(V)(1−), 10CI



M 355.2 (ion)

Square-pyramidal anion. Synth. from $TcOCl_4^{\ominus}$ + thiooxalate in Me_2CO.

Tetrabutylammonium salt: [73396-10-8].

Burgundy-maroon cryst. (Me_2CO aq.). Mp 126-127°.

Ph_4As salt: [73396-09-5].

Red-brown cryst. (Me_2CO aq.).

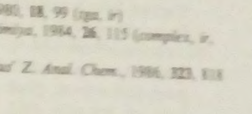
Davison, A. *et al. Inorg. Chem.*, 1980, **19**, 1988 (*synth, uv*)
Colmanet, S.F. *et al. Inorg. Chim. Acta*, 1988, **147**, 173 (*cryst struct*)

$C_4O_8Pd^{2\ominus}$ IC-004590

Bis(oxalato)palladate(*II*)(2−), 8CI

Bis(ethanedioato(2−)-O,O')palladate(II)(2−), 9CI

[15226-60-5]



M 282.4 (ion)

Prob. square planar struct. Formation of Pd metal on light irradiation gives potential photographic applications.

Di-K salt: [28766-27-0].

Degree of hydration uncertain. Sol. H_2O.

[15651-95-3, 36425-78-2, 38682-90-5]

Vèzes, M., *Bull. Soc. Chim. Fr.*, 1899, **21**, 172 (*synth*)
Nagase, K. *et al. Bull. Chem. Soc. Jpn.*, 1973, **46**, 144 (*thermal anal*)
Nakayama, K. *et al. Bull. Chem. Soc. Jpn.*, 1984, **57**, 2930 (*uv, mcd*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **6**, 113, 117 (*use*)

$C_4O_8Pt^{2\ominus}$ IC-004591

Bis(oxalato)platinate(*II*)(2−), 8CI

Bis(ethanedioato)platinate(2−), 9CI

[36444-17-4]

As Bis(dithiooxalato)platinate(*II*), IC-004585 with

X = O

M 371.1 (ion)

Stacked struct. Particular interest in 1-D electrical conductance of many salts when partially oxidised (Krogmann's salts). Cations may be hydrated on complexed metals, $NH_4^{\oplus}$ or alkyl derivatives or other organic ions. Such complexes are colloquially known as KOP, MgOP, CoOP, etc.

K salt, dihydrate: [14244-64-5].

Yellow solid, becomes violet on partial oxidation.

▷ TT3780000.

Cu salt, 3.5 hydrate: [21136-03-8].

Red solid.

[35371-78-9, 40729-78-0]

Krogmann, K. *et al. Chem. Ber.*, 1966, **99**, 3402 (*synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **6**, 139 (*struct, props*)

C_4O_8Pu IC-004592

Plutonium(*IV*) oxalate

$Pu(C_2O_4)_2$

M 415.0

Dihydrate:

$C_4H_4O_{10}Pu$ M 451.1

Green cryst.

Dihydrate, Me_2CO solvate: Bright pink cryst. Obtd. by Me_2CO washing of dihydrate. Slowly dec. to dihydrate.

Hexahydrate: [74280-13-0].

$C_4H_{16}O_{18}Pu$ M 523.1

Yellow-green cryst. Insol. H_2O. Undergoes auto-radiolytic dec. to $PuOCO_3$. Isomorphous with U analogue.

Bis(urea) complex: [89743-21-5].

$C_6H_8N_4O_{10}Pu$ M 535.2

Cryst. + $2H_2O$.

Mandleberg, C.J. *et al. J. Chem. Soc.*, 1961, 2464 (*anal*)
Jenkins, I.L. *et al. Chem. Ind. (London)*, 1963, 35.
Jenkins, I.L. *et al. J. Inorg. Nucl. Chem.*, 1965, **27**, 77, 81.
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, C, 236 (*rev*)
Cleveland, J.M., *The Chemistry of Plutonium*, American Nuclear Society, 1979, 400 (*rev*)
Nissen, D.A., *J. Therm. Anal.*, 1980, **18**, 99 (*tga, ir*)
Andryushin, V.G. *et al. Radiokhimiya*, 1984, **26**, 115 (*complex, ir, dta*)
Kanellakopulos, B. *et al. Fresenius' Z. Anal. Chem.*, 1986, **323**, 818 (*synth*)

C_4O_8Th IC-004593

Thorium(*IV*) oxalate

Bis(ethanedioato)thorium

[2040-52-0]

$Th(C_2O_4)_2$

M 408.0

Usually obt. as hexahydrate. Can be pptd. quantitatively and ignited to afford ThO_2 for gravimetric analysis.

Hexahydrate: [16788-62-8].

$C_4H_{12}O_{14}Th$ M 516.1

White cryst. Sl. sol. H_2O; sol. in solns. of alkali metal oxalates. At 110° forms dihydrate; above 160° in vacuo forms anhydrous oxalate.

Bressat, R. *et al. Bull. Soc. Chim. Fr.*, 1963, 464 (*props*)
Bressat, R. *et al. J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1265.
Inorg. Synth., 1966, **8**, 43 (*synth*)
Molodkhin, A.K. *et al. Zh. Neorg. Khim.*, 1968, **13**, 2117; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1095 (*synth*)
Subramanian, M.S. *et al. J. Inorg. Nucl. Chem.*, 1969, **31**, 3789 (*dta*)
Kharitonov, Y.Y. *et al. Zh. Neorg. Khim.*, 1969, **14**, 339; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 174 (*ir*)

$C_4O_8Ti^{\ominus}$ IC-004594

Bis(oxalato)titanate(*III*)(1−), 8CI

Bis[ethanedioato(2−)-O,O']titanate(III)(1−), 10CI

[31226-07-0]

$[Ti(C_2O_4)_2]^{\ominus}$

M 223.9 (ion)

Proposed struct. contains Ti chains with bridging oxalato groups. Salts may be used as the photosensitive layer in printed circuit board manuf.

K salt: [15655-84-2].

Synth. by dehydrating the dihydrate. Catalyses polyester formation. Paramagnetic; μ_{eff} = 1.64μ_B (292K), 1.53μ_B (80K).

K salt, dihydrate: [65900-51-8].
Synth. by adding oxalic acid and $TiCl_3$ to H_2O then adding $K_2C_2O_4$. Orange solid. Paramagnetic; μ_{eff} = 1.77μ_B (292K), 1.60μ_B (80K).

[27459-12-7]

Eve, D.J. *et al, J. Chem. Soc. A*, 1966, 1183 (*synth, ua-vis, ir, K salts*)
Kalinnikov, V.T. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1969, 2836; *CA*, **72**, 84291t (*magnetism*)
Japan. Pat., 70 27 837, (1970); *CA*, **73**, 131560n (*use, polyester catal*)
Drew, M.G.B. *et al, Inorg. Chim. Acta*, 1977, **25**, L111 (*synth, cryst struct, ir, ua-vis, dihydrate*)

C_4O_8U IC-004595

Uranium(*IV*) oxalate

[63057-31-8]

$U(C_2O_4)_2$

M 414.0
Blue-violet cryst. Sl. sol. H_2O. Dec. above 400° to UO_2.

Dihydrate:
$C_4H_4O_{10}U$ M 450.0
Formed from hexahydrate at 110°. Cryst. Sl. sol. H_2O. Isomorphous with Th and Pu analogues.

Hexahydrate: [65665-14-7].
Pptd. when oxalic acid added to U(*IV*) soln. Air-stable green-yellow cryst. (dark green microcryst.). Sl. sol. H_2O, sol. hot conc. HCl. Sol. oxalates to form $U(C_2O_4)_4^{4\ominus}$. Loses $4H_2O$ at 110° or *in vacuo* at r.t. All H_2O lost at 200°. Isomorphous with Pu analogue.

Inorg. Synth., 1950, **3**, 166 (*synth*)
Bressat, R. *et al, Bull. Soc. Chim. Fr.*, 1963, 464.
Bressat, R. *et al, J. Chim. Phys.*, 1963, **60**, 1265.
Jenkins, I.L. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 81 (*struct*)
Awasthi, S.K. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 3805 (*synth, ir*)
Hanuza, J. *et al, Acta Phys. Pol. A*, 1974, **45**, 885 (*ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1251 (*hexahydrate*)

$C_4O_8Ti^{2\ominus}$ IC-004596

Bis(oxalato)oxotitanate(*IV*)(2−)

Bis[ethanedioato(2−)-O,O′]oxotitanate(IV)(2−), *11CI*

M 239.9 (ion)
Square based pyramid. Various salts used in the manuf. of titanates for use as dielectrics, thermistors, ceramics and piezoelectric devices.

Di-K salt: [14481-26-6].
Catalyst for polym. of esters.

Ba salt: [14523-21-8].
C_4BaO_9Ti M 377.2
Synth. by adding EtOH soln. of oxalic acid to aq. $Ba(NO_3)_2/TiO(NO_3)_2$ soln. Starting material for manuf. of barium titanate. Forms a tetrahydrate.

Pb salt: [27111-57-5].
C_4O_9PbTi M 447.1
Synth. by adding $TiOCl_2$ and $PbCl_2$ to hot aq. $H_2C_2O_4$. Starting material for manuf. of lead titanate-based thermistors.

[14263-62-8]

Kudaka, K. *et al, Am. Ceram. Soc. Bull.*, 1982, **61**, 1236 (*synth, Ba salt hydrate*)
Balachandran, R. *et al, Mater. Chem. Phys.*, 1984, **10**, 287 (*synth, thermal dec, Pb salt*)
Yamamura, H. *et al, Ceram. Int.*, 1985, **11**, 17 (*synth, Ba salt*)
Fr. Pat., 2 507 373, (1986); *CA*, **105**, 193857c (*synth, use, Pb salt*)

$C_4O_9V^{2\ominus}$ IC-004597

Bis(oxalato)oxovanadate(*IV*)(2−)

Bis[ethanedioato(2−)-O,O′]oxovanadate(IV)(2−), *11CI*

[17569-94-7]

M 242.9 (ion)
Square pyramidal. Various alkali metal and alkaline earth metal salts may be synth. similarly. A number of hydrates also is known.

Di-Na salt: [82861-62-9].
Synth. by reduction of V_2O_5 by aq. $H_2C_2O_4$ + $Na_2C_2O_4$. Blue solid + $2H_2O$ (H_2O). This and the Li salt dec. to M_3VO_4 on heating (*cf.* Ba salt).

Ba salt: [65690-25-7].
Synth. by reducing V_2O_5 with aq. $H_2C_2O_4$ and adding a soluble Ba salt. Blue solid (H_2O). Dec. to $BaVO_3$ on heating in an inert atm.

Di-NH_4 salt: [82873-25-4].
Synth. from NH_4VO_3 with $H_2C_2O_4$ and aq. $(NH_4)_2C_2O_4$. Blue solid + $1H_2O$ (H_2O). Dec. on heating to V_2O_5.

Murthy, H.S. *et al, Indian J. Chem., Sect. A*, 1977, **15**, 863 (*synth, thermal dec, alkaline earth salts*)
Saikali, Y. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1982, **294**, 839 (*synth, thermal dec, alkali metal salts*)

$C_4O_9Zr^{2\ominus}$ IC-004598

Bis(oxalato)oxozirconate(*IV*)

Bis[ethanedioato(2−)-O,O′]oxozirconate(IV)(2−), *11CI*

M 283.2 (ion)
Various salts have been used to prepare $MZrO_3$ in high purity.

Ba salt: [42863-88-7].
Formed by metathesis of corresp. NH_4 salt. Forms thixotropic suspensions. White solid. Forms a number of hydrates.

Cd salt: [82930-15-2].
Synth. by adding aq. $ZrCl_4$ and $CdCl_2$ to hot aq. oxalic acid and precipitating with EtOH. White solid.

Bis-Pyridinium salt: [97059-19-3].
Synth. from aq. $ZrCl_4$ + PyHCl + oxalic acid. White solid.

Sharma, A.K. *et al, Thermochim. Acta*, 1982, **56**, 221; 1985, **93**, 101 (*synth, ir, thermal dec*)
Fr. Pat., 2 570 373, (1986); *CA*, **105**, 193857c (*use*)
Gangadevi, T. *et al, Monatsh. Chem.*, 1987, **117**, 21 (*synth, thermal anal, Ba salt*)

$C_4O_{10}Os^{2\ominus}$ IC-004599

Bis(oxalato)dioxoosmate(*VI*)(2−)

M 398.2 (ion)
Struct. is assigned to point group D_{2h} with oxygen atoms in *trans*-position. Synth. from $[OsO_2(OH)_4]^{2\ominus}$ + oxalic acid. K, Cs, NH_4, Bu_4N salts known.

Di-K salt: [22827-17-4].
Synth. by reacting K_2OsO_4 with potassium tetroxalate soln. Brown solid + $5H_2O$.

Griffith, W.P., *J. Chem. Soc.*, 1964, 245 (*synth, ir*)
Griffith, W.P., *J. Chem. Soc. A*, 1969, 211 (*synth, ir*)
Hanuza, J. *et al, Acta Phys. Pol. A*, 1970, **38**, 563 (*ir*)
Preetz, W. *et al, Z. Naturforsch., B*, 1983, **38**, 183.
Linko, I.V. *et al, Zh. Neorg. Khim.*, 1983, **28**, 1520 (*pe*)
Packard, A.B. *et al, J. Nucl. Med.*, 1987, **28**, 1571 (*use*)

$C_4O_{10}Ru^{2\ominus}$ IC-004600

Bis(oxalato)dioxoruthenate(*VI*)(2−)

Bis[ethanedioato(2−)-O,O′]dioxoruthenate(2−), *9CI*

M 309.1 (ion)
trans-Octahedral anion.

Di-Cs salt: [38883-00-0].
Prepd. by treating a soln. of RuO_4 in CCl_4 with a soln. of $Cs_2[C_2O_4]$ in aq. oxalic acid at 0°. Green diamagnetic salt. Ir ν_{RuO_2} 838 cm^{-1}.

Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)

$C_4O_{10}Ti^{2\ominus}$ IC-004601

Bis[oxalato(2−)-*O,O′*]peroxytitanate(*IV*)(2−)

Bis[ethanedioato(2−)-O,O′]peroxytitanate(IV)(2−), *11CI*

M 255.9 (ion)
Prob. struct. shown.

Di-K salt: [12075-33-1].
Synth. by adding excess H_2O_2 to an aq. soln. of $K_2TiO(oxalate)_2$. Yellow solid. Insol. EtOH, Et_2O; sol. H_2O.

Patel, C.C. *et al, J. Inorg. Nucl. Chem.*, 1963, **25**, 1155 (*synth, ir*)
Griffith, W.P., *J. Chem. Soc.*, 1964, 5248 (*synth, ir, raman*)
Nour, E.M. *et al, Inorg. Chim. Acta*, 1986, **117**, 45 (*raman*)

$C_4O_{10}V^{3\ominus}$ IC-004602

Bis(oxalato)dioxovanadate(*V*)(3−)

Bis[ethanedioato(2−)-O,O′]dioxovanadate(V)(3−), *11CI*

[14971-68-7]

M 258.9 (ion)
Octahedral.

cis-form [56556-47-9]

Tri-K salt: [54203-19-9].
Synth. from aq. KVO_3, $K_2C_2O_4$ and $H_2C_2O_4$. Yellow cryst. + $3H_2O$ (H_2O). Previously described as red due to the presence of impurities.

Ba salt (2:3): [36426-92-3].
Synth. from NH_4VO_3, $H_2C_2O_4$, $(NH_4)_2C_2O_4$ and $Ba(NO_3)_2$ in H_2O. Solid + $6H_2O$.

Tri-NH_4 salt: [14516-26-8].
Synth. from NH_4VO_3, $(NH_4)_2C_2O_4$ and $H_2C_2O_4$ in H_2O. Solid + $2H_2O$.

[34788-02-8]

Gopalkrishnan, J. *et al, CA*, 1970, **76**, 135163v (*synth*)
Drew, M.G.B. *et al, Can. J. Chem.*, 1974, **52**, 2184 (*synth, cryst struct*)
Misra, B.N. *et al, Chem. Phys.*, 1978, **31**, 95 (*synth*)
Stomberg, R., *Acta Chem. Scand., Ser. A*, 1986, **40**, 168 (*synth, cryst, struct*)

$C_4O_{11}V^{3\ominus}$ IC-004603

Bis(oxalato)oxoperoxyvanadate(*V*)(3−)

Bis[ethanedioato(2−)-O,O′]oxoperoxyvanadate(V)(3−), *11CI*

M 274.9 (ion)
Pentagonal bipyramidal.

Tri-K salt, monohydrate: [65057-99-0].
Synth. by mixing solns. of KVO_3 and $H_2C_2O_4$ in H_2O_2. Image intensifier in colour photography. Use of $K_2C_2O_4$ in the synth. yields $K_3[VO(O_2)_2C_2O_4]$.

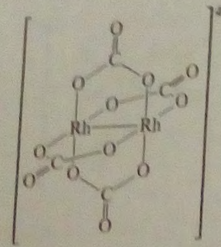
Tri-K salt, hemihydrate: [103728-92-3].

Japan. Pat., 77 79 928, (1977); *CA*, **87**, 209509p (*use*)
Schwendt, P. *et al, Z. Anorg. Allg. Chem.*, 1980, **466**, 232 (*synth, ir, K salt*)
Schwendt, P., *Collect. Czech. Chem. Commun.*, 1983, **48**, 248 (*ir*)
Stomberg, R., *Acta Chem. Scand., Ser. A*, 1986, **40**, 168 (*synth, cryst struct, hemihydrate*)

$C_4O_{12}Rh_2^{4\ominus}$ IC-004604

Tetrakis[μ-[carbonato(2−)-*O*:*O*']]dirhodate(*II*)(4−), 10CI

Tetracarbonatodirhodate(II)(4−)



M 445.8 (ion)

Prob. struct. shown. Synth. e.g. from a fresh soln. of $Rh_2^{4\oplus}$ (aq.) and excess aq. carbonate ion under inert atm. Addition of $Na^\oplus$ or $K^\oplus$ leads to pptn. of derivs. Diamagnetic.

Tetra-K salt (hydrate): [53078-64-1].
No phys. props. reported.

Bis[ethylenediammonium(2+)] salt: Synth. by metathesis of corresp. K_4 salt. Lilac solid + $4H_2O$.

Tetrakis-guanidinium salt: Synth. by ion-exchange of corresp. K_4 salt. Medium blue solid + $4H_2O$.

Wilson, C.R. *et al, Inorg. Chem.*, 1975, **14**, 405 (*synth, electrochem, ir, uv-vis*)
Shchelokov, R.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 770 (*synth, ir*)

$C_5BrCrO_5^\ominus$ IC-004605

Bromopentacarbonylchromate(1−), 9CI

[14911-72-9]

$[(OC)_5CrBr]^\ominus$ (C_{4v})

M 271.9 (ion)

Me_4N salt: [14780-93-9].
Orange cryst.

Abel, E.W. *et al, J. Chem. Soc.*, 1963, 2068 (*synth*)
Knoll, L., *J. Organomet. Chem.*, 1979, **182**, 77 (*props*)
Chatt, J. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 2032.
Cotton, F.A. *et al, Inorg. Chem.*, 1981, **20**, 578 (*props*)
Nixon, J.F. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 199 (*props*)

$C_5BrHgMnO_5$ IC-004606

(Bromomercury)pentacarbonylmanganese, 9CI

(Bromomercurio)pentacarbonylmanganese

[17524-66-2]

$BrHgMn(CO)_5$

M 475.4

Synth. from $Hg[Mn(CO)_5]_2$ and $HgBr_2$. Colourless needles (MeOH). Mp 172° dec. Ir ν_{CO} 2107m, 2046w, 2021vs cm^{-1} ($CHCl_3$).

Hieber, W. *et al, Chem. Ber.*, 1960, **93**, 455 (*synth, ir*)
Brier, P.N. *et al, J. Chem. Soc. A*, 1967, 1889 (*ir*)
Bower, L.M. *et al, J. Chem. Soc. A*, 1968, 706 (*ir*)
Hsieh, A.T.T., *Int. J. Mass Spectrom. Ion Phys.*, 1971, **7**, 319 (*ms*)

$C_5BrIrN_5^{3\ominus}$ IC-004607

Bromopentakis(cyano-*C*)iridate(*III*)(3−)

Bromopentacyanoiridate(III)

$[Ir(CN)_5Br]^{3\ominus}$

M 402.2 (ion)

Tri-K salt: [42893-04-9].
Synth. from $[Ir(CN)_5H_2O]^{2\ominus}$ and KBr. Sol. H_2O.

Hexaamminecobalt(3+) salt: [42893-08-3].
$C_5H_{18}BrCoIrN_{11}$ M 563.3
Synth. from the K salt and $[Co(NH_3)_6]Cl_3$. Sol. H_2O.

Geoffroy, G.L. *et al, Inorg. Chem.*, 1974, **13**, 430 (*synth, ir, uv*)

C_5BrMnO_5 IC-004608

Bromopentacarbonylmanganese, 10CI, 9CI, 8CI

[14516-54-2]

$MnBr(CO)_5$ (C_{4v})

M 274.8

Synth. from $Mn_2(CO)_{10}$ and Br_2 in CS_2. Orange-yellow cryst. Mod. sol. org. solvs. $Subl._{0.05}$ 50°. Dimerises slowly in soln. with loss of CO.

Abel, E.W. *et al, J. Chem. Soc.*, 1959, 1501 (*synth, props*)
Kaesz, H.D. *et al, J. Am. Chem. Soc.*, 1967, **89**, 2844 (*ir*)
Connor, J.A. *et al, J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 1754.
Aime, S. *et al, Transition Met. Chem.*, 1976, **1**, 177 (*cmr*)
Inorg. Synth., 1979, **19**, 160 (*synth*)

C_5BrO_5Re IC-004609

Bromopentacarbonylrhenium, 9CI, 8CI

Rhenium pentacarbonyl bromide

[14220-21-4]

$Re(CO)_5Br$

M 406.1

Synth. from $Re(CO)_5I$ or $Re_2(CO)_{10}$ and Br_2. Air stable white cryst. (by subl.). $Subl._{0.2}$ 85-90°. Ir ν_{CO} 2150w, 2050s, 2015w, 1990m, cm^{-1} (CCl_4).

Kirkham, W.J. *et al, J. Chem. Soc.*, 1965, 550 (*synth*)
Kaesz, H.D. *et al, J. Am. Chem. Soc.*, 1967, **89**, 2844 (*ir*)
Junk, G.A. *et al, J. Am. Chem. Soc.*, 1968, **90**, 5758 (*ms*)
Keeling, G. *et al, J. Chem. Soc. A*, 1971, 3143 (*ir*)
Colton, R. *et al, Aust. J. Chem.*, 1972, **25**, 9 (*synth, ir*)
Hall, M.B., *J. Am. Chem. Soc.*, 1975, **97**, 2057 (*uv*)
Higginson, B.R. *et al, J. Chem. Soc., Faraday Trans. 2*, 1975, **71**, 1913 (*pe*)
Webb, M.J. *et al, J. Organomet. Chem.*, 1975, **93**, 119 (*cmr*)
Al-Takhim, G. *et al, J. Organomet. Chem.*, 1983, **259**, 313 (*props*)
Inorg. Synth., 1985, **23**, 44 (*synth*)

C_5BrO_5Tc IC-004610

Bromopentacarbonyltechnetium, 10CI

[15841-97-1]

$(OC)_5TcBr$ (C_{4v})

M 318.8

Yellow cryst. by subl. Sublimes *in vacuo*.

[78514-64-4]

Bor, G. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 1073 (*props*)
Behrens, R.G. *et al, J. Less-Common Met.*, 1978, **61**, 321 (*props*)
Micheis, E.D. *et al, Inorg. Chem.*, 1981, **20**, 3445 (*synth*)
Kruglov, A.A. *et al, Zh. Neorg. Khim.*, 1981, **26**, 960 (*cryst struct*)
Findeisen, M. *et al, Inorg. Chim. Acta*, 1987, **128**, L15 (*Tc-99 nmr*)

$C_5Br_2GaMnO_5$ IC-004611

Pentacarbonyl(dibromogallio)manganese

[21255-48-1]

$Br_2GaMn(CO)_5$

M 424.5

Synth. from $Mn_2(CO)_{10}$ and Ga_2Br_4. Pale-yellow air-sensitive cryst. (CH_2Cl_2). Insol. pentane.

Hoyano, J. *et al, Inorg. Nucl. Chem. Lett.*, 1968, **4**, 201 (*synth, ms*)

$C_5Br_3GeMnO_5$ IC-004612

Pentacarbonyl(tribromogermyl)manganese, 9CI

[17770-03-5]

$Br_3GeMn(CO)_5$

M 507.3

MnGe 244 pm. Yellow cryst. Mp 165-166°. Ir ν_{CO} 2126m, 2047s, 2036m cm^{-1} (cyclohexane). Subl. *in vacuo*.

Nesmeyanov, A.N. *et al, Izv. Akad. Scl. USSR, Ser. Sci. Khim.*, 1960, 160; 1966, 160 (*synth*)
Gapotchenko, N.I. *et al, J. Organomet. Chem.*, 1970, **23**, 525 (*struct*)
Gapokchenko, N.I. *et al, Zh. Strukt. Khim.*, 1971, **12**, 571 (*struct*)
Onaka, S., *J. Inorg. Nucl. Chem.*, 1974, **36**, 1721 (*ir*)

$C_5Br_3MnO_5Sn$ IC-004613

Pentacarbonyl(tribromostannyl)manganese

[16165-08-5]

$Br_3SnMn(CO)_5$

M 553.4

Moisture-sensitive pale yellow cryst. (CCl_4). Mp 146-148°, Mp 145-147°. Ir ν_{CO} 2122, 2060, 2043, 2037 cm^{-1} (cyclohexane).

Gorsich, R.D., *J. Am. Chem. Soc.*, 1962, **84**, 2486 (*synth*)
Jetz, W. *et al, Inorg. Chem.*, 1966, **5**, 2217 (*ir*)
Onaka, S. *et al, Bull. Chem. Soc. Jpn.*, 1971, **44**, 726 (*mössbauer, Mn-55 nmr*)
Kume, Y. *et al, J. Magn. Reson.*, 1973, **10**, 58 (*nqr*)
Onaka, S. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 258 (*mössbauer, ir*)

$C_5CdIMnO_5$ IC-004614

Pentacarbonyl(iodocadmio)manganese

[31386-09-1]

$ICdMn(CO)_5$

M 434.3

Synth. from $Cd[Mn(CO)_5]_2$ and CdI_2 in Me_2CO or MeOH. Air- and light-sensitive bright-yellow cryst.(MeOH). Ir ν_{CO} 2076, 2005, 1976 cm^{-1}. Corresp. Br analogue also known.

Hsieh, A.T.T. *et al, J. Chem. Soc. A*, 1971, 729 (*synth, ir*)

$C_5CeO_{15}^{6\ominus}$ IC-004615

Pentakis(carbonato)cerate(*IV*)(6−)

Pentacarbonatocerate(IV)(6−)

$[Ce(CO_3)_5]^{6\ominus}$

M 440.1 (ion)

Hexa-Na salt: [57341-10-3].
$C_5CeNa_6O_{15}$ M 578.0
Yellow cryst. + $12H_2O$. 10-Coord. with bidentate carbonates: irregular decahexahedron.

Hexa-guanidinium salt: [51407-08-0].
Piezoelectric. Yellow cryst. + $4H_2O$. 10-Coord. with bidentate carbonates: irregular decahexahedron.

[57965-84-1, 58081-59-7]

Dervin, J. *et al, Bull. Soc. Chim. Fr.*, 1973, 2634 (*synth, dta*)
Voliotis, S. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2607, 2620 (*cryst struct*)
Voliotis, S. *et al, Rev. Chim. Minér.*, 1977, **14**, 441 (*synth, ir, struct*)
Jolivet, J.P. *et al, J. Mol. Struct.*, 1980, **60**, 93; 1982, **79**, 403 (*ir, raman*)

$C_5ClCrO_5^\ominus$ IC-004616

Pentacarbonylchlorochromate(1−), 9CI

[14911-56-9]

$[(OC)_5CrCl]^\ominus$

M 227.5 (ion)
Octahedral.

Et_4N salt: [14780-95-1].
Yellow cryst. Sol. $CHCl_3$, insol. Et_2O.

Bis(triphenylphosphine)iminium salt: [65650-76-2].
Yellow cryst. Ir ν_{CO} 2059, 1926, 1854 cm^{-1}.

Abel, E.W. *et al, J. Chem. Soc.*, 1963, 2068 (*synth*)
Cotton, F.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 398 (*props*)
Grillone, M.D., *Transition Met. Chem.*, 1981, **6**, 93 (*synth*)

$C_5ClHgMnO_5$ IC-004617

Pentacarbonyl(chloromercury)manganese, 10CI, 9CI

[17524-65-1]

$ClHgMn(CO)_5$

M 431.0

Synth. from $Hg[Mn(CO)_5]_2$ and $HgBr_2$ in Me_2CO. Colourless needles (MeOH). Mp 170° dec. (163° dec.). Ir ν_{CO} 2109m, 2048w, 2024vs cm^{-1} ($CHCl_3$).

Hieber, W. *et al, Chem. Ber.*, 1960, **93**, 455 (*synth, ir*)
Brier, P.N. *et al, J. Chem. Soc. A*, 1967, 1889 (*ir*)
Bower, L.M. *et al, J. Chem. Soc. A*, 1968, 706 (*ir*)
Hsieh, A.T.T., *Int. J. Mass Spectrom. Ion Phys.*, 1971, **7**, 319 (*ms*)

$C_5ClIrN_5^{3\ominus}$ IC-004618

Chloropentakis(cyano-*C*)iridate(*III*)(3−)

Chloropentacyanoiridate(III)

$[Ir(CN)_5Cl]^{3\ominus}$ (C_{4v})

M 357.7 (ion)

Tri-K salt: [42893-03-8].
Synth. from $[Ir(CN)_5H_2O]^{2\ominus}$ and KCl. Appearance not descr. Sol. H_2O.

Hexaamminecobalt(3+) salt: [42893-09-4].
$C_5H_{18}ClCoIrN_{11}$ M 518.8
Synth. from the K salt and $[Co(NH_3)_6]Cl_3$. Appearance not descr. Sol. H_2O.

Geoffroy, G.L. *et al, Inorg. Chem.*, 1974, **13**, 430 (*synth, ir, uv*)

C_5ClMnO_5 IC-004619

Pentacarbonylchloromanganese, 10CI

Chloropentacarbonylmanganese

[14100-30-2]

$MnCl(CO)_5$ (C_{4v})

M 230.4

Synth. from $Mn_2(CO)_{10}$ and Cl_2 in CCl_4. Pale-yellow light-sensitive cryst. Mod. sol. org. solvs. Subl.$_{0.1}$ 40°. Dimerises slowly in soln. with loss of CO.

Abel, E.W. *et al*, *J. Chem. Soc.*, 1959, 1501 (*synth, props*)
Kaesz, H.D. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2844 (*ir*)
Greene, P.T. *et al*, *J. Chem. Soc. A*, 1971, 1559 (*cryst struct*)
Connor, J.A. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 1754.
Inorg. Synth., 1979, **19**, 159 (*synth*)

IC-004620

C_5ClMnO_9

Pentacarbonyl(perchlorato-*O*)manganese, 10Cl

[66034-78-4]

$Mn(OClO_3)(CO)_5$

M 294.4
Synth. from $MnBr(CO)_5$ + $AgClO_4$ in CH_2Cl_2. Useful for obtaining other $[Mn(CO)_5L]^{\oplus}$ cations (L = R_3P, Py, RCN, OH_2). Reacts with $CHCl_3$ to give $MnCl(CO)_5$ at r.t. Ir ν_{CO} 2168, 2085, 2034 cm^{-1}.

Wimmer, F.L. *et al*, *Aust. J. Chem.*, 1978, **31**, 267 (*synth*)
Snow, M.R. *et al*, *Inorg. Chim. Acta*, 1980, **44**, L189 (*props*)

IC-004621

$C_5ClN_5Rh^{3\ominus}$

Chloropentakis(cyano-*C*)rhodate(*III*)(3 –), 9Cl

Chloropentacyanorhodate(III)

$[Rh(CN)_5Cl]^{3\ominus}$ (C_{4v})

M 268.4 (ion)
Tri-K salt: [42892-94-4].
Appearance not recorded. Sol. H_2O.

Geoffroy, G.L. *et al*, *Inorg. Chem.*, 1974, **13**, 430 (*synth, ir, uv*)

IC-004622

C_5ClO_5Re

Pentacarbonylchlororhenium, 9Cl, 8Cl

Chloropentacarbonylrhenium. Rhenium pentacarbonyl chloride

[14099-01-5]

$Re(CO)_5Cl$ (C_{4v})

M 361.7
Synth. from $Re_2(CO)_{10}$ and Cl_2 or uv irradiation or from $Re(CO)_5I$ and Cl_2. White air-stable cryst. (C_6H_6). Subl.$_{0.3}$ 80-85°, Subl. 140°. Ir ν_{CO} 2130w, 2055s, 2020w, 1985m cm^{-1} (CCl_4).

Kirkham, W.J. *et al*, *J. Chem. Soc.*, 1965, 550 (*synth*)
Kaesz, H.D. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2844 (*ir*)
Junk, G.A. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5758 (*ms*)
Colton, R. *et al*, *Aust. J. Chem.*, 1972, **25**, 9 (*synth, ir*)
Higginson, B.R. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1975, **71**, 1913 (*pe*)
Wrighton, M.S. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1111 (*uv*)
Inorg. Synth., 1985, **23**, 41 (*synth, ir*)

IC-004623

C_5ClO_5Tc

Pentacarbonylchlorotechnetium, 10Cl

Chloropentacarbonyltechnetium

[15841-98-2]

$(OC)_5TcCl$ (C_{4v})

M 274.4
Colourless cryst.

Hileman, J.C. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2453 (*synth*)
Behrens, R.G., *J. Less-Common Met.*, 1978, **61**, 321 (*props*)
Kruglov, A.A. *et al*, *Zh. Neorg. Khim.*, 1981, **26**, 960 (*cryst struct*)

IC-004624

$C_5Cl_3GeMnO_5$

Pentacarbonyl(trichlorogermyl)manganese, 9Cl

[14768-39-9]

$Cl_3GeMn(CO)_5$

M 373.9
Air-stable white cryst. (hexane). Insol. H_2O; sol. org. solvs. Mp 168.5-169°. Ir ν_{CO} 2128m, 2048s, 2038m cm^{-1} (cyclohexane). Subl. *in vacuo*.

Nesmeyanov, A.N. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1965, 1309; 1966, 160 (*synth*)
Bancroft, G.M. *et al*, *Inorg. Chem.*, 1973, **12**, 728 (*Mn-55 nmr*)
Onaka, S., *CA*, 1973, **25**, 133 (*raman*)
Onaka, S., *J. Inorg. Nucl. Chem.*, 1974, **36**, 1721 (*ir*)

IC-004625

$C_5Cl_3MnO_5Si$

Pentacarbonyl(trichlorosilyl)manganese, 9Cl

[38194-30-8]

$Cl_3SiMn(CO)_5$

M 329.4
Synth. by heating $SiHCl_3$ and $Mn_2(CO)_{10}$ in a sealed tube. Moisture-sensitive white cryst. Mp 130-131°. Ir ν_{CO} 2123, 2035 cm^{-1} (cyclohexane).

[15488-10-5]

Jetz, W. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2773 (*synth, ir*)
Bancroft, G.M. *et al*, *Inorg. Chem.*, 1973, **12**, 728 (*Mn-55 nmr*)
Onaka, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 258 (*mössbauer, ir*)
Krentz, R. *et al*, *Inorg. Chem.*, 1985, **24**, 2976 (*Si-29 nmr*)

IC-004626

$C_5Cl_3MnO_5Sn$

Pentacarbonyl(trichlorostannyl)manganese, 9Cl

[16165-09-6]

$Cl_3SnMn(CO)_5$

M 420.0
Synth. from $Ph_3SnMn(CO)_5$ and Cl_2 in CCl_4. Moisture-sensitive white cryst. (CCl_4). Mp 168° dec., Mp 173-174°. Ir ν_{CO} 2126, 2046, 2039 cm^{-1} (cyclohexane).

[17635-52-8]

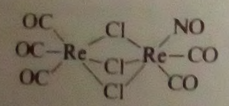
Gorsich, R.D., *J. Am. Chem. Soc.*, 1962, **84**, 2486 (*synth*)
Brier, P.N. *et al*, *J. Chem. Soc. A*, 1967, 1889 (*ir, raman*)
Onaka, S., *Bull. Chem. Soc. Jpn.*, 1971, **44**, 726 (*mössbauer*)
Bancroft, G.M. *et al*, *Inorg. Chem.*, 1973, **12**, 728 (*Mn-55 nmr*)
Kume, Y. *et al*, *J. Magn. Reson.*, 1973, **10**, 58 (*nqr*)
Onaka, S., *Bull. Chem. Soc. Jpn.*, 1975, **48**, 319 (*struct*)

IC-004627

$C_5Cl_3NO_6Re_2$

Pentacarbonyltri-μ-chloronitrosyldirhenium, 9Cl

[37402-69-0]



M 648.8
Synth. from $[Re(CO)_4Cl]_2$ and NO. Mod. air-stable light-orange cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2, CCl_4, C_6H_6, reacts with EtOH. Ir ν_{CO} 2113m, 2047vs, 1946s; ν_{NO} 1813m cm^{-1} (CCl_4).

Norton, J.R. *et al*, *Inorg. Chem.*, 1973, **12**, 485 (*synth, ir*)
Inorg. Synth., 1976, **16**, 36 (*synth, ir, raman*)

IC-004628

$C_5CoN_5^{4\ominus}$

Pentakis(cyano-*C*)cobaltate(4 –), 8Cl

Pentacyanocobaltate(1)

$[Co(CN)_5]^{4\ominus}$

M 189.0 (ion)
Formed by pulse radiolysis of $Co^{2\oplus}/CN^{\ominus}$ aq. solns. Soon dec. to Aquapentakis(cyano-*C*)cobaltate(2 –), IC-004660.

Venerable, G.D. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 2176 (*kinetics*)

IC-004629

$C_5CoN_5^{3\ominus}$

Pentakis(cyano-*C*)cobaltate(3 –), 10Cl

Pentacyanocobaltate(3 –)

[14971-18-7]

$[Co(CN)_5]^{3\ominus}$

M 189.0 (ion)
Square pyramidal anion, may have H_2O coord. in aq. solns. Catalyst for hydrogenation of alkenes, dienes, dienones, Schiff bases, cyanation of alkenes and for deuterium-water exchange. Undergoes oxidative addition with O_2, C_2F_4, C_2H_2, SO_2 etc. Formed in solns. of $[Co(H_2O)_6]^{3\oplus}$ with excess $CN^{\ominus}$. Paramagnetic.

Tri-Li salt: [24803-72-3].
$C_{10}Co_2Li_4N_{10}$ M 419.6
Violet-red cryst. Dimeric: $Li_6[Co_2(CN)_{10}]$.
Tri-K salt: [15415-02-8].
$C_5CoK_3N_5$ M 306.3
Fuel-cell electrolyte, catalyst in hydrogenation of coal. Brown solid. Ir ν_{CN} 2129, 2077, 2042 cm^{-1}.
Tri-K salt, dimer:
$C_{10}Co_2K_6N_{10}$ M 612.6
Violet cryst. (H_2O). Ir ν_{CN} 2128, 2120, 2110, 2079 cm^{-1}.
Tris-Et$_4$N salt: [38141-18-3].
Yellow cryst. (DMF).
Tris-tetrabutylammonium salt: [38141-19-4].
Yellow cryst. (hexamethylphosphoramide).

[37473-63-5]

Kwiatek, J., *Catal. Rev.*, 1967, **1**, 37 (*use*)
Alexander, J.J. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 3356 (*esr*)
Pregaglia, G. *et al*, *Discuss. Faraday Soc.*, 1968, 110 (*synth*)
Coulton, K.G. *et al*, *Inorg. Chem.*, 1968, **7**, 392 (*uv*)
Reinstein, J.G. *et al*, *Inorg. Chem.*, 1969, **8**, 2499.
White, D.A. *et al*, *Inorg. Chem.*, 1972, **11**, 2160 (*synth, uv*)
Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 158 (*struct, ir, raman*)
Ohkubo, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 1114 (*use*)
Brown, L.D., *Inorg. Chem.*, 1975, **14**, 2590 (*cryst struct, synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1989, **4**, 648 (*reactions*)

IC-004630

$C_5CoN_5O_2^{3\ominus}$

Pentakis(cyano-*C*)(dioxygen)cobaltate(*III*)(3 –), 9Cl

(Dioxygen)pentacyanocobaltate(III)(3 –)

$[O\text{-}O\text{-}Co(CN)_5]^{3\ominus}$

M 221.0 (ion)
Model complex for O_2 transport systems.
Tris-Et$_4$N salt: [38141-20-7].
Red-brown cryst.

White, D.A. *et al*, *Inorg. Chem.*, 1972, **11**, 2160 (*synth, ir, esr*)
Brown, L.D. *et al*, *Inorg. Chem.*, 1975, **14**, 2595 (*synth, cryst struct*)

IC-004631

$C_5CoN_6O^{3\ominus}$

Pentakis(cyano-*C*)nitrosylcobaltate(3 –), 11Cl, 10Cl

Pentacyanonitrosylcobaltate(3 –)

[33290-75-4]

$[Co(CN)_5(NO)]^{3\ominus}$

M 219.0 (ion)
Approx. octahedral anion.
Tri-K salt: [14099-02-6].
Yellow cryst. solid + $2H_2O$. V. sol. H_2O. Toyuki suggests possible formulation as $K_3[(CN)_5Co(N_2O_2)Co(CN)_5].4H_2O$. Stable only in strongly alkaline solns. Ir ν_{CN} 2205, 2128, ν_{NO} ~1130, 1050, 980 cm^{-1}. Diamagnetic.

[90668-64-7, 117151-91-4]

Nast, R. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **309**, 283 (*synth*)
Toyuki, H., *Spectrochim. Acta, Part A*, 1971, **27**, 985 (*ir, synth*)

IC-004632

$C_5CoN_8^{3\ominus}$

Azidopentakis(cyano-*C*)cobaltate(3 –), 11Cl, 10Cl

Azidopentacyanocobaltate(III)

[19400-45-4]

$[CoN_3(CN)_5]^{3\ominus}$

M 231.0 (ion)
Approx. octahedral coord. about Co. Co—C_{ax} 189, C—N_{ax} 151.1 pm. Azide is linear and asymmetric. CoN—NN 120.4; CoNN—N 115.6 pm.
Tri-K salt: [14705-99-8].
Golden needles (dil. HCl/MeOH). Sol. H_2O. Ir ν_{NNN} 2070, 1300, 604, ν_{CoNN} 2130; ν_{Co-C} 418, 378 cm^{-1} (mineral oil).
Tri-K salt, dihydrate: [82861-86-7].
Synth. from $[Co(NH_3)_5N_3]Cl_2$, KCN and $CoCl_2.6H_2O$ catalyst. Yellow plates (H_2O).
Pentaammineaquacobalt(3+) salt: [102941-70-8].
Pentaammineaquacobalt(3+) azidopentakis(cyano-C) cobaltate(3 –)
Solid. Sol. H_2O. Isostructural with $[Co(NH_3)_6][CoCN_6]$. Possesses trigonally distorted CsCl type lattice. Ir ν_{CN} 2180, 2115, ν_{NNN} 2040 cm^{-1} (KBr).
Tetraamminediaquacobalt(3+) salt: [110635-30-8]. cis-*Tetraamminediaquacobalt(3+) azidopentakis(cyano-C) cobaltate(3 –)*
Solid. Sol. H_2O. Ages to form polymeric material with μ-cyano bridging. Possesses a trigonally distorted CsCl type lattice.
Tris-tetrabutylammonium salt: [33848-07-6].
Cryst. Sol. H_2O. Ir ν_{NNN} 2035, 2020, 625, 598, ν_{CoNN} 2106; ν_{Co-C} 415 cm^{-1} (mineral oil).

Gray, H.B. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 3364 (*synth, uv-vis, ir*)
Castellano, E.E. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2239 (*cryst struct, K dihydrate*)
Casabó, J. *et al*, *Inorg. Chem.*, 1986, **25**, 3166 (*double salt, ir, Co-59 nmr, uv-vis, struct*)
Flor, T. *et al*, *Polyhedron*, 1987, **6**, 1563 (*double salt, uv-vis, struct, ir*)

IC-004633

$C_5CrIO_5^{\ominus}$

Pentacarbonyliodochromate(1 –), 10Cl

[14780-98-4]

$[(OC)_5CrI]^{\ominus}$ (C_{4v})

M 318.9 (ion)
Et_4N salt: Orange cryst.

$MePh_3P$ salt: [76309-27-8].
Orange cryst.

Abel, E.W. *et al*, *J. Chem. Soc.*, 1963, 2068 (*synth*)
Organomet. Synth., 1965, **1**, 122 (*synth*)
Grim, S. *et al*, *Inorg. Chem.*, 1980, **19**, 2475 (*props*)
Angelici, R.J. *et al*, *Inorg. Chem.*, 1980, **19**, 3853 (*props*)
Magomedov, G.K. *et al*, *Zh. Obshch. Khim.*, 1980, **50**, 2623 (*props*)

$C_5CrN_5S_5^{3\ominus}$ IC-004634

Pentakis(thiocyanato-*N*)chromate(*II*)(3−), 10CI
Pentaisothiocyanatochromate(II)(3−)

$[Cr(NCS)_5]^{3\ominus}$

M 342.4 (ion)
Square pyramidal, H_2O molecule may complete octahedron.

Tri-Na salt: [73440-47-8].
Synth. from aq. $CrCl_2.4H_2O$ and $NaSCN.H_2O$. Hygroscopic, unstable, air-sensitive deep lilac-blue cryst. Sol. Me_2CO, EtOAc. Degree of hydration uncertain. μ_{eff} = 4.5μ_B (r.t.).

Larkworthy, L.F. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 262 (*magnetism, uv, ir, synth*)

$C_5CrN_6O^{3\ominus}$ IC-004635

Pentakis(cyano-*C*)nitrosylchromate(3−), 11CI, 10CI, 9CI
Pentacyanonitrosylchromate(3−)
[25360-58-1]

$[Cr(NO)(CN)_5]^{3\ominus}$ (C_{4v})

M 212.0 (ion)
$CN^\ominus$ may be replaced by H_2O and other ligands. N—O 121, Cr—NO 171, Cr—C_{eq} (av.) 203.3, Cr—C_{ax} 207.5 pm, angle: CrNO 176°.

Tri-K salt, monohydrate: [67740-35-6].
Synth. by reduction of K_2CrO_4 in strongly alkaline KCN with hydroxylamine in excess. Bright green cryst. (EtOH aq.). μ_{eff} = 1.87μ_B (298K). Ir ν_{NO} 1637, ν_{CN} 2120, ν_{CrN} 620 cm^{-1}.

Tris(ethylenediamine)cobalt(III) *salt:* [55991-02-1].
$C_{11}H_{24}CoCrN_{13}O$ M 451.3
Bright yellow cryst. Ir ν_{NO} 1660 cm^{-1}.

Tris(ethylenediamine)chromium(III) *salt:* [74438-21-4].
Bright yellow cryst. Ir ν_{NO} 1670 cm^{-1}.

Tri-NH_4 salt: [60255-53-0].
Synth. by neutralisation with ammonia of $H_3[Cr(CN)_5NO]$ from tri-K salt. Green solid. Sol. H_2O, MeOH.

[14100-08-4]

Enemark, J.H. *et al*, *Inorg. Chem.*, 1970, **9**, 2397 (*cryst struct*)
Horvath, A. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **42**, 195 (*thermal dec*)
Inorg. Synth., 1985, **23**, 182 (*synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 786 (*rev*)

$C_5CrO_5^{2\ominus}$ IC-004636

Pentacarbonylchromate(2−), 9CI

$[Cr(CO)_5]^{2\ominus}$

M 192.0 (ion)
Trigonal bipyramidal struct.

Di-Li salt:
$C_5CrLi_2O_5$ M 205.9
Sol. THF. Less stable than Na salt. Ir ν_{CO} 1810vs, 1762s, 1690s, 1654m cm^{-1}(THF).

Di-Na salt: [52154-81-1].
$C_5CrNa_2O_5$ M 238.0
Air- and moisture-sensitive yellow powder, gives greenish soln. in THF. Dec. readily. Ir ν_{CO} 1817vs, 1766vs cm^{-1} (THF).

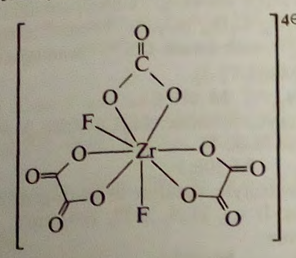
Di-Cs salt: [57127-95-4].
$C_5CrCs_2O_5$ M 457.8
Reactive anion.

[51233-19-3]

Behrens, H. *et al*, *Z. Anorg. Allg. Chem.*, 1960, **306**, 94 (*props*)
Behrens, H. *et al*, *Chem. Ber.*, 1967, **96**, 2220 (*props*)
Behrens, H. *et al*, *Z. Naturforsch., B*, 1973, **18**, 276 (*synth*)
Ellis, J.E. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 7825 (*synth*)
Ellis, J.E. *et al*, *J. Organomet. Chem.*, 1975, **97**, 79 (*props*)
Ellis, J.E. *et al*, *Inorg. Chem.*, 1977, **16**, 1357 (*synth, props*)
Ellis, J.E. *et al*, *Organometallics*, 1985, **4**, 1354 (*improved synth, ir*)
Organomet. Synth., 1986, **3**, 35 (*synth, ir*)

$C_5F_2O_{11}Zr^{4\ominus}$ IC-004637

(Carbonato)difluorobis(oxalato)zirconate(*IV*)(4−)
[*Carbonato*(2−)-O,O′]*bis*[*ethanedioato*(2−)-O,O′]*difluorozirconate*(IV)(4−), *11CI*



M 365.2 (ion)
Bicapped trigonal prism. In view of the ease of dehydration there must be some doubt as to the unique nature of the tetra- and penta-hydrates. Synth. from $K_4Zr(C_2O_4)_4.5H_2O$, KF and $KHCO_3$ in aq. soln.

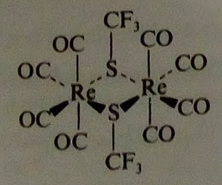
Tetra-K salt, tetrahydrate: [93451-11-7].
White solid (H_2O).

Tetra-K salt, pentahydrate: [66329-61-1].
White solid (H_2O).

Medkov, M.A. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1978, 270; *CA*, **88**, 163087q (*synth, cryst struct, pentahydrate*)
Eiberman, M.F. *et al*, *Koord. Khim.*, 1984, **10**, 1266; *CA*, **101**, 238415t (*synth, cryst struct, tetrahydrate*)

$C_5F_3O_4ReS$ IC-004638

Tetracarbonyl(trifluoromethanethiolato)rhenium



M 399.3
Dimeric. Synth. from $Re(CO)_5I$ and $Hg(SCF_3)_2$ or $Re(CO)_5Br$ and CF_3SAg. Ir ν_{CO} 2110vs, 2030vs, 2018vs, 1995vs cm^{-1} (cyclohexane).

Dimer: [25031-36-1]. *Octacarbonylbis*[*μ*-(*trifluoromethanethiolato*)]*dirhenium, 8CI*
$C_{10}F_6O_8Re_2S_2$ M 798.6
White cryst. by fractional subl. Mp 129°. $Subl._{0.1}$ 70°.

King, R.B. *et al*, *Inorg. Chem.*, 1969, **8**, 2540 (*synth, ir, F-19 nmr*)
Grobe, J. *et al*, *J. Fluorine Chem.*, 1976, **8**, 145 (*synth, ir, F-19 nmr*)

$C_5F_5MnO_6Te$ IC-004639

Pentacarbonyl(pentafluorohydroxytellurato-*O*)manganese, 11CI
[90414-49-6]

$Mn(OTeF_5)(CO)_5$ (C_{4v})

M 433.5
Mn—O 204 pm; angle MnOTe 139.3°. Synth. from $MeMn(CO)_5$ and $HOTeF_5$ in CH_2Cl_2 at 22°. Orange cryst. (CH_2Cl_2); stable under N_2, dec. in CH_2Cl_2.

Abney, K.D. *et al*, *Inorg. Chem.*, 1984, **23**, 1994 (*synth, ir, ms, uv, F-19 nmr, cryst struct*)

$C_5F_6O_5Re_2$ IC-004640

Pentacarbonyl-μ-fluoropentafluorodirhenium, 9CI
[41884-64-4]

$F_5ReFRe(CO)_5$

M 626.4
Can be regarded either as covalent adduct (preferred) or as $ReF_6^\ominus$ salt of $Re(CO)_5^\oplus$. Synth. from $Re_2(CO)_{10}$ and ReF_6 in HF. V. moisture-sensitive orange platelets.

Bruce, D.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 321 (*synth, cryst struct*)

$C_5FeN_5O_3S^{5\ominus}$ IC-004641

Pentakis(cyano-*C*)[sulfito(2−)-*S*]ferrate(*II*)(5−), 9CI
Pentacyanosulfitoferrate(II)

$[Fe(CN)_5(SO_3)]^{5\ominus}$

M 266.0 (ion)
Octahedral anion. Labile $[Fe(CN)_5L]$ deriv.

Penta-Na salt: [12169-60-7].
Synth. from $Na_2[Fe(CN)_5(NO)]$ + alkaline Na_2SO_3. Yellow cryst. + H_2O. There is uncertainty about the degree of hydration.

[75559-97-6]

Chadwick, B.M. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1966, **8**, 83 (*rev, bibl*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, N.Y., 1976, 138 (*rev, bibl*)
Jagner, S. *et al*, *Acta Chem. Scand., Ser. B*, 1980, **36**, 96 (*cryst struct*)
Passoja, A. *et al*, *Finn. Chem. Lett.*, 1980, 119, 122 (*uv, ir, synth*)

$C_5FeN_6O^{2\ominus}$ IC-004642

Pentakis(cyano-*C*)nitrosylferrate(2−), 9CI
Pentacyanonitrosylferrate(III). *Nitroprusside*
[15078-28-1]

$[Fe(CN)_5NO]^{2\ominus}$

M 215.9 (ion)
Best viewed as an $NO^\oplus$ complex. Aq. solns. dec. in light. Salts usually diamagnetic, but may change to high spin at low temps.

Di-Na salt: [13755-38-9]. *Sodium nitroferricyanide. Sodium nitroprusside, USAN. Nipride. Nitropress. Acetest. Nipruss*
$C_5FeN_6Na_2O$ M 261.9
Antihypertensive drug. Reagent for detn. of many organic compds. Standard for ^{57}Fe Mössbauer. Analytical reagent for $SH^\ominus$. Ruby red rhombic cryst. + $2H_2O$. Ir ν_{NO} 1947 cm^{-1}.
▷ LJ8925000.

Di-K salt: [14709-57-0].
Cryst. + $1H_2O$. Sol. H_2O.

[14323-53-6, 14402-89-2, 104493-97-2]

Manoharan, P.T. *et al*, *Inorg. Chem.*, 1963, **2**, 1043 (*synth*)
Chadwick, B.M. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1966, **8**, 83 (*rev, bibl*)
Brown, D.R., *Inorg. Chim. Acta*, 1971, **9**, 314 (*mössbauer*)
Malin, J.M. *et al*, *Inorg. Chem.*, 1975, **14**, 2924 (*nmr, cmr*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, N.Y., 1976 (*rev, bibl*)
Mohai, B. *et al*, *Acta Chim. Acad. Sci. Hung.*, 1977, **92**, 271 (*synth*)
Castellano, E.E. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1725, 1728 (*cryst struct*)
Rucki, R., *Anal. Profiles Drug Subst.*, 1977, **6**, 487; 1986, **15**, 781 (*rev, props*)
Ivankovitch, A.D. *et al*, *Int. Anesthesiol. Clin.*, 1978, **16**, 1 (*rev, pharmacol*)
Long, J.C. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1627 (*mössbauer*)
Bottomley, F. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2193 (*cryst struct*)
Posse, M.E.G. *et al*, *Inorg. Chem.*, 1984, **23**, 948 (*cryst struct*)

$C_5FeN_6O_2^{4\ominus}$ IC-004643

Pentakis(cyano-*C*)(nitrito-*N*)ferrate(*II*)(4−)
Pentacyano(*nitro*-N)*ferrate*(II)
[15003-01-7]

$[Fe(CN)_5(NO_2)]^{4\ominus}$

M 231.9 (ion)
Octahedral anion. In equilibrium with Pentakis(cyano-*C*)nitrosylferrate(2−), IC-004642 in aq. soln.: $[Fe(CN)_5(NO)]^{2\ominus} + 2OH^\ominus \rightleftharpoons [Fe(CN)_5(NO_2)]^{4\ominus}$.

Tetra-Na salt: [14099-03-7].
Synth. from conc. NaOH (aq.) or aq. methanolic $[Fe(CN)_5(NO)]^{2\ominus}$ at 2°. Yellow solid. Ir ν_{CN} 2060 cm^{-1}.

Tetra-K salt: [14709-58-1].
From $[Fe(CN)_5NO]^{2\ominus}$ + KOH in MeOH. Mustard yellow.

Chadwick, B.M. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1966, **8**, 83 (*rev, bibl*)
Swinehart, J.H. *et al*, *Inorg. Chem.*, 1966, **5**, 573 (*uv, equilibrium*)
West, D.X., *J. Inorg. Nucl. Chem.*, 1967, **29**, 1163 (*ir*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, London, 1976, 134 (*rev, bibl*)
Eaton, D.R. *et al*, *Inorg. Chem.*, 1985, **24**, 1424 (*synth*)
Butler, A.R., *Inorg. Chem.*, 1985, **24**, 2931 (*cmr*)

C_5FeO_4S IC-004644

Tetracarbonyl(thiocarbonyl)iron
(*Carbonothioyl*)*tetracarbonyliron, 10CI*
[66517-47-3]

$Fe(CO)_4CS$

M 211.9
Yellow-orange volatile light-sensitive oil at r.t., bright-yellow cryst. at −78°.

Petz, W. *et al*, *J. Organomet. Chem.*, 1978, **146**, C23; 1981, **205**, 203 (*synth, ir, cmr, ms*)

IC-004645

$C_5FeO_4S_2$

(Carbon disulfide)tetracarbonyliron, 8CI

[19194-19-5]

$Fe(CO)_4(CS_2)$

M 244.0

Synth. and used *in situ*. Sol. CS_2.

Baird, M.C. *et al*, *J. Chem. Soc. A*, 1967, 2037 (*synth, ir*)

IC-004646

C_5FeO_5

Pentacarbonyliron

Iron carbonyl, 9CI, 8CI. Iron pentacarbonyl

[13463-40-6]

$Fe(CO)_5$

M 195.8

Fluxional trigonal bipyramidal molecule. Commercially available. Catalyst for carbonylation and polymn. Used in manuf. of pure iron. Pale yellow viscous liq. Sol. hexane. d_{18}^{18} 1.47. Fp −20° to −19.5°. Bp_{749} 102.8°. Dec. at 180° → Fe + CO.

▷ Highly toxic by inhalation and skin absorption, TLV 0.08. Pyrophoric in air. NO4900000.

Ewens, R.V.G. *et al*, *Trans. Faraday Soc.*, 1939, **35**, 681 (*cryst struct*)
McDowell, R.S., *CA*, 1972, **76**, 89720 (*ir*)
Grobe, J. *et al*, *Z. Naturforsch., B*, 1973, **28**, 691 (*synth*)
Hagen, A.P. *et al*, *Inorg. Chem.*, 1978, **17**, 1369 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 59, 1979, **B3** (*rev, bibl*)
Inorg. Synth., 1989, **25**, 151.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 367.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 2010.

IC-004647

$C_5HCoN_5^{3\ominus}$

Pentakis(cyano-*C*)hydrocobaltate(3−), 10CI

Pentacyanohydrocobaltate(3−), 8CI. Hydridopentacyanocobaltate(3−)

[17168-56-8]

$[HCo(CN)_5]^{3\ominus}$

M 190.0 (ion)

Homogenous hydrogenation catalyst for the reduction of conjugated dienes to olefins. Useful under micellar and phase transfer conditions.

Tri-Li salt: [24803-73-4].
Characterised in soln. only.

Tri-K salt: [18117-30-1].
Characterised in soln. only.

Griffith, W.P. *et al*, *J. Chem. Soc.*, 1959, 2757 (*synth, pmr, uv*)
Pregaglia, G. *et al*, *Discuss. Faraday Soc.*, 1968, **46**, 110 (*synth, use*)
Lim, H.S. *et al*, *Inorg. Chem.*, 1971, **10**, 103 (*synth*)
Venerable, G.D. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 2176 (*synth, bibl*)
Funabiki, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2945 (*ir*)
Clase, H.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2546 (*raman*)
Reger, D.L., *Adv. Chem. Ser.*, 1979, 173 (*use, rev*)

IC-004648

$C_5HCoN_5O^{3\ominus}$

Pentakis(cyano-*C*)hydroxycobaltate(*III*)(3−), 9CI

Pentacyanohydroxocobaltate(III)

[16893-73-5]

$[Co(CN)_5(OH)]^{3\ominus}$

M 206.0 (ion)

Prepd. in aq. soln. Not isol.

Scandola, M.A.R. *et al*, *Inorg. Chim. Acta*, 1981, **54**, L159 (*synth, photochem*)
Wrighton, M. *et al*, *Inorg. Chem.*, 1973, **12**, 1707 (*synth, uv, photochem*)

IC-004649

$C_5HCrN_5O^{3\ominus}$

Pentakis(cyano-*C*)hydroxychromate(*III*)(3−), 11CI, 10CI

[88886-75-3]

$[Cr(OH)(CN)_5]^{3\ominus}$ (C_{4v})

M 199.0 (ion)

Tri-K salt: [77983-16-5].
Synth. from hot aq. $[CrCl(NH_3)_5]Cl$ and KCN followed by purif. on Sephadex gel. Orange-yellow cryst. (H_2O).

[34276-13-6]

Jeftic, L. *et al*, *J. Phys. Chem.*, 1971, **75**, 2381 (*synth, uv*)
Sakabe, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 1253 (*synth, ir, uv*)
Marchaj, A. *et al*, *Polyhedron*, 1983, **2**, 485, 1281 (*photochem*)

IC-004650

$C_5HIrN_5^{3\ominus}$

Pentakis(cyano-*C*)hydroiridate(3−), 11CI

Pentacyanohydridoiridate(III)

$[Ir(CN)_5H]^{3\ominus}$ (C_{4v})

M 323.3 (ion)

Tri-K salt: [17685-53-9].
White solid (aq. MeOH). Sol. H_2O.

Krogmann, K. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1967, **6**, 881 (*synth, uv, props*)
Mockford, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 717 (*synth, ir, raman, cmr*)

IC-004651

C_5HMnO_5

Pentacarbonylhydromanganese, 9CI

Pentacarbonylmanganese hydride. Manganese hydrocarbonyl. Hydridopentacarbonylmanganese

[16972-33-1]

$HMn(CO)_5$ (C_{4v})

M 195.9

Synth. from $Na[Mn(CO)_5]$ and H_3PO_4 in THF. Liq. Mp −20°. pK_a 15.1. Sublimes *in vacuo*. Stable to 50°. Ir ν_{CO} 2012 cm^{-1} (MeCN).

▷ Poisonous vapour.

Inorg. Synth., 1963, **7**, 198 (*synth*)
Organomet. Synth., 1965, **1**, 158 (*synth*)
Edgell, W.F. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 5451 (*synth*)
Calderazzo, F. *et al*, *J. Chem. Soc. A*, 1967, 154 (*nmr*)
Edgell, W.F. *et al*, *Inorg. Chem.*, 1969, **8**, 1103 (*ir*)
La Placa, S. *et al*, *Inorg. Chem.*, 1969, **8**, 1928 (*cryst struct*)
McNeill, E.A. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 6243 (*synth, struct*)
McKinney, R.J. *et al*, *Inorg. Chem.*, 1979, **18**, 3413.
Moore, E.J. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2257 (*ir, props*)

IC-004652

C_5HMnO_5S

Pentacarbonylmercaptomanganese, 9CI

[59390-73-7]

$HSMn(CO)_5$

M 228.0

Readily loses CO to give di-, tri-, and tetranuclear species. Synth. from either $[MnSH(CO)_4]_2$ or $[Mn(CO)_3SH]_4$ and CO. Formed in soln. Ir ν_{CO} 2120s, 2035vs, 2004m cm^{-1} (CCl_4).

Küllmer, V. *et al*, *Chem. Ber.*, 1976, **109**, 1560 (*synth, ir*)

IC-004653

$C_5HN_5Rh^{3\ominus}$

Pentakis(cyano-*C*)hydrorhodate(3−), 10CI

Pentacyanohydrorhodate(3−), 8CI. Hydridopentakis(cyano)rhodate(3−)

$[RhH(CN)_5]^{3\ominus}$

M 234.0 (ion)

Tri-Na salt: [33916-04-0].
Sol. MeOH.

Tri-K salt: [19610-72-1].
White cryst. (MeOH). Sol. H_2O, MeOH. V. hygroscopic.

[33916-05-1]

Krogmann, K. *et al*, *J. Organomet. Chem.*, 1968, **11**, P27 (*synth, ir, uv, pmr*)
Whitesides, G.M. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 4980 (*synth, pmr, cmr*)
Jewsbury, R.A. *et al*, *J. Chem. Soc. A*, 1971, 2847 (*synth, uv, ir, pmr, raman*)
Mockford, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 717 (*synth, ir, raman, pmr, cmr, N-14 nmr*)

IC-004654

$C_5HNbO_5^{2\ominus}$

Pentacarbonylhydroniobate(2−), 11CI

Hydridopentacarbonylniobate(2−)

$[HNb(CO)_5]^{2\ominus}$

M 233.9 (ion)

Salts are thermally unstable. Na salt less stable than Et_4N salt. More easily handled starting material than $[Nb(CO)_5]^{3\ominus}$.

Bis-Et_4N salt: [91265-44-0].
Synth. by reaction of an ammoniacal soln. of $Na_3[Nb(CO)_5]$ with 1 equiv. EtOH in THF. Orange cryst. Dec. in polar solvs. at r.t.

Warnock, G.F.P. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5016 (*synth, use, ir, pmr, Nb-93 nmr*)

IC-004655

$C_5HO_5Os^{\oplus}$

Pentacarbonylhydroosmium(1+), 8CI

$[HOs(CO)_5]^{\oplus}$

M 331.2 (ion)

Hexafluorophosphate: [30306-42-4].
White solid.

Lewis, J. *et al*, *J. Chem. Soc. A*, 1970, 2967 (*synth, ir, pmr*)

IC-004656

C_5HO_5Re

Pentacarbonylhydrorhenium, 9CI, 8CI

Hydridopentacarbonylrhenium. Pentacarbonylrhenium(I) *hydride. Hydrogen pentacarbonyl rhenate(1−)*

[16457-30-0]

$HRe(CO)_5$ (C_{4v})

M 327.2

Synth. from $NaRe(CO)_5$ and H_3PO_4. Air- and moisture-sensitive colourless liq. Insol. H_2O; sol. common org. solvs. Mp 12.5°. Bp *ca.* 100° (extrap.). pK_a 21.1. With radical initiators gives $^{\cdot}Re(CO)_5$ useful in synth. of substituted complexes. Dec. at *ca.* 100° to H_2 + $Re_2(CO)_{10}$. Ir ν_{CO} 2012 cm^{-1} (MeCN). Ir ν_{CO} 2131vw, 2041vw, 2016vs, 2007s, 1983vw, 1965vw; ν_{Re-H} 1832vw cm^{-1} (hexane).

Beck, W. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **308**, 23 (*synth, ir*)
Braterman, P.S. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2851 (*ir*)
Byers, B.H. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 2527 (*synth, ir, pmr, uv*)
Miles, W.J. *et al*, *J. Organomet. Chem.*, 1977, **131**, 93 (*synth, ir*)
Moore, E.J. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2257 (*ir, pKa*)

IC-004657

$C_5HO_5Ru^{\ominus}$

Pentacarbonylhydroruthenium(*II*)(1+), 10CI

[79160-22-8]

$[RuH(CO)_5]^{\ominus}$ (C_{4v})

M 242.1 (ion)

Synth. by extracting a hexane soln. of $Ru(CO)_5$ with CO-saturated conc. H_2SO_4. Pale yellow soln. – indefinitely stable at r.t. under CO. Sol. conc. H_2SO_4.

Deeming, A.J. *et al*, *J. Chem. Soc. A*, 1970, 2967 (*synth, pmr*)
Yarrow, P. *et al*, *J. Organomet. Chem.*, 1981, **215**, 115 (*synth, cmr, pmr*)

IC-004658

$C_5HO_5Ta^{2\ominus}$

Pentacarbonylhydrotantalate(2−), 11CI

Hydridopentacarbonyltantalate(2−)

$[HTa(CO)_5]^{2\ominus}$

M 322.0 (ion)

Salts are thermally unstable. Na salt less stable than Et_4N salt. More easily handled starting material than $[Ta(CO)_5]^{3\ominus}$.

Bis-Et_4N salt: [91239-64-4].
Synth. by reaction of an ammoniacal soln. of $Na_3[Ta(CO)_5]$ with 1 equiv. EtOH in THF. Orange-red cryst. Dec. in polar solvs. at r.t.

Warnock, G.F.P. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5016 (*synth, use, ir, pmr*)

IC-004659

$C_5HO_5V^{2\ominus}$

Pentacarbonylhydrovanadate(2−), 11CI

Hydridopentacarbonylvanadate(2−)

$[HV(CO)_5]^{2\ominus}$

M 192.0 (ion)

Salts are thermally unstable. Na salt less stable than Et_4N salt. More convenient starting material than $[V(CO)_5]^{3\ominus}$.

Et_4N salt: [91239-62-2].
Synth. by reaction of an ammoniacal soln. of $Na_3[V(CO)_5]$ in THF with 1 equiv. EtOH then $[Et_4N]BH_4$. Bright-yellow cryst. Dec. in polar solvs. at r.t.

Warnock, G.F.P. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5016 (*synth, use, ir, pmr, V-51 nmr*)

IC-004660

$C_5H_2CoN_5O^{2\ominus}$

Aquapentakis(cyano-*C*)cobaltate(2−), 8CI

Aquapentacyanocobaltate(III)(2−)

[14842-83-2]

$[Co(CN)_5OH_2]^{2\ominus}$

M 207.0 (ion)

Di-K salt: Yellow solid.

Haim, A. *et al, Inorg. Chem.*, 1962, **1**, 573 (*reactions, kinetics*)
Bayston, J.H. *et al, Aust. J. Chem.*, 1963, **16**, 954 (*synth*)
Valentine, J.S. *et al, J. Am. Chem. Soc.*, 1971, **93**, 1111 (*uv*)

IC-004661

$C_5H_2FeN_5O^{3\ominus}$

Aquapentakis(cyano-*C*)ferrate(*II*)(3−), 9CI

Aquapentacyanoferrate(II)(*3*−). *Aquoferrocyanide*

[18497-51-3]

$[Fe^{II}(CN)_5(OH_2)]^{3\ominus}$

M 203.9 (ion)
Octahedral anion. Obt. variously by: (1) Hydrol. of $[Fe(CN)_6]^{4\ominus}$ in presence of light, heat or dilute acid, (2) reduction of $[Fe(CN)_5(NO)]^{2\ominus}$ in alkaline soln., (3) hydrol. of $[Fe(CN)_5(NH_3)]^{3\ominus}$ in presence of ascorbic acid. Used in spectrophotometric analysis. Synthetic intermed. Photocatalyst for reduction. Samples rarely pure. Redox active, photolabile. Sol. H_2O. May be reduced to blue $[Fe(CN)_5(H_2O)]^{2\ominus}$.

Tri-Na salt: [14100-31-3].
Useful precursor and redox agent. Light yellow deliquescent powder + $1H_2O$. Contains $[Fe_2(CN)_{10}]^{6\ominus}$ as well as $Na_2[Fe(CN)_5(OH_2)]$.

Hofmann, K.A., *Justus Liebigs Ann. Chem.*, 1900, **312**, 1 (*synth*)
Asperger, S. *et al, J. Chem. Soc.*, 1955, 449 (*synth*)
Chadwick, B.M. *et al, Adv. Inorg. Chem. Radiochem.*, 1966, **8**, 83 (*rev, bibl*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, N.Y., 1976 (*rev, bibl*)
Compr. Coord. Chem., Pergamon, 1987, **4**, 1179 (*rev, bibl*)
Beck, M.T., *Pure Appl. Chem.*, 1987, **59**, 1703 (*stability*)

IC-004662

$C_5H_2IrN_5O^{2\ominus}$

Aquapentakis(cyano-*C*)iridate(*III*)(2−), 9CI

Aquapentacyanotridate(III)

[42893-00-5]

$[Ir(CN)_5OH_2]^{2\ominus}$

M 340.3 (ion)
Octahedral. Present in aq. soln. Not isol.

Geoffroy, G.L. *et al, Inorg. Chem.*, 1974, **13**, 430 (*synth, uv*)

IC-004663

$C_5H_2MnO_4P$

Pentacarbonyl(phosphino)manganese, 9CI

[35126-88-6]

$H_2PMn(CO)_5$

M 227.9
Poorly characterised. Synth. from SiH_3PH_2 and $MnBr(CO)_5$. Ir ν_{CO} 2020s, 1960m cm^{-1} (cyclohexane).

Sabherwal, I.H. *et al, Inorg. Nucl. Chem. Lett.*, 1972, **8**, 27 (*synth, ir*)

IC-004664

$C_5H_2N_5ORh^{2\ominus}$

Aquapentakis(cyano-*C*)rhodate(*III*)(2−), 9CI

Aquapentacyanorhodate(III)

[42892-92-2]

$[Rh(CN)_5(OH_2)]^{2\ominus}$ (C_{4v})

M 251.0 (ion)
Present in ionic form in aq. soln. Not isol.

Geoffroy, G.L. *et al, Inorg. Chem.*, 1974, **13**, 430 (*synth, uv*)

IC-004665

$C_5H_3AsCrO_5$

(Arsine)pentacarbonylchromium, 8CI

Pentacarbonylarsinechromium

[29454-58-8]

$(OC)_5CrAsH_3$ (C_{4v})

M 269.9
Yellow cryst. Mp 90-70°.

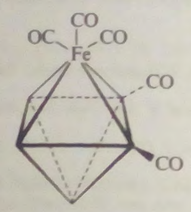
Dobson, G.R. *et al, Inorg. Chim. Acta*, 1967, **1**, 287 (*synth*)
Fischer, E.O. *et al, Chem. Ber.*, 1970, **103**, 1815; 1971, **104**, 986 (*synth*)

IC-004666

$C_5H_3B_2FeO_5$

Tricarbonyl[(2,3,4,5-η)-dicarbonyltrihydropentaborato(2−)]iron, 10CI

[61525-93-7]



M 252.9
Orange solid or red liq. Mp ~5°.

Ulman, J.A. *et al, J. Chem. Soc., Chem. Commun.*, 1976, 632 (*synth, ms, ir, nmr, pmr*)
Ulman, J.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 456 (*pe*)

IC-004667

$C_5H_3CrNO_5$

Amminepentacarbonylchromium, 9CI

[15228-27-0]

$(OC)_5CrNH_3$ (C_{4v})

M 209.0
Yellow cryst. Mp 150°.

Behrens, H. *et al, Chem. Ber.*, 1964, **97**, 433 (*synth*)
Strohmeier, W. *et al, Chem. Ber.*, 1966, **99**, 3419 (*synth*)
Lloyd, D.R. *et al, J. Chem. Soc., Faraday Trans. 2*, 1974, 1418 (*pe*)
Sellmann, D. *et al, Angew. Chem.*, 1975, **87**, 772 (*props*)
Sellmann, D. *et al, J. Organomet. Chem.*, 1976, **111**, 303 (*props*)

IC-004668

$C_5H_3CrO_5Sb$

Pentacarbonyl(stibine)chromium, 8CI

[32356-12-0]

$(OC)_5CrSbH_3$ (C_{4v})

M 316.8
Orange-yellow cryst. Mp 44°.

Fischer, E.O. *et al, Chem. Ber.*, 1971, **104**, 986 (*synth, ir, nmr*)

IC-004669

$C_5H_3FeN_6^{3\ominus}$

Amminepentakis(cyano-*C*)ferrate(*II*)(3−)

[13717-31-2]

$[Fe(CN)_5(NH_3)]^{3\ominus}$ (C_{4v})

M 202.9 (ion)
NH_3 ligand readily hydrolyses; complex is also subject to aerial oxidation. Synth. e.g. from nitroprusside + NH_3 soln. or by reduction of (4−) ion with Na/Hg. Used in

determination of biological molecules; photoelectrocatalyst; electrode modifier for CO chem. Low spin Fe(*II*) complex, but converts to high spin at high pressures.

Tri-Na salt: [14099-05-9].
$C_5H_3FeN_6Na_3$ M 271.9
Common salt used for numerous analytical and catalytic purposes. Pale yellow. Forms tri- and hexahydrates. K salt also known.

Fe(III) salt: [63016-10-4].
$C_5H_3Fe_2N_6$ M 258.8
Synth. from $FeCl_3$ + $Na_3[Fe(CN)_5(NH_3)]$. Pale blue solid.

[23388-75-2]

Hoffmann, K.A., *Z. Anorg. Allg. Chem.*, 1895, **10**, 262; 1896, **12**, 146 (*synth*)
Ungarelli, A., *Gazz. Chim. Ital.*, 1925, **55**, 118 (*synth*)
*Gmelin Handbook Inorg. Chem., Syst. No.*59, 1929, **B**, 732 (*rev*)
Herington, E.F.G. *et al, J. Chem. Soc.*, 1955, 3555 (*ir*)
Kenney, D.J., *J. Inorg. Nucl. Chem.*, 1961, **20**, 75 (*synth, reactivity*)
Maltz, H. *et al, J. Org. Chem.*, 1971, **36**, 363 (*derivs*)
Toma, H.E. *et al, Inorg. Chem.*, 1973, **12**, 1039 (*kinetics of dissoc*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1657 (*synth*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, 1976, 129 (*rev, bibl*)
Inoue, H. *et al, Z. Anorg. Allg. Chem.*, 1981, **483**, 75 (*mössbauer, esca*)
Griffith, W.P. *et al, Inorg. Chim. Acta*, 1987, **26**, 179 (*ir, nmr*)

IC-004670

$C_5H_3FeN_6^{2\ominus}$

Amminepentakis(cyano-*C*)ferrate(*III*)(2−)

[19413-98-0]

$[Fe(CN)_5(NH_3)]^{2\ominus}$

M 202.9 (ion)
Octahedral anion. Obt. by oxidation of corresp. ferrate(3−).

Di-Na salt: [15928-32-2].
Yellow cryst. + $2H_2O$ (EtOH aq.), sl. dec. in air.

*Gmelin Handbook Inorg. Chem., Syst. No.*59, 1929, **B**, 732 (*rev, bibl*)
Herington, E.F.G. *et al, J. Chem. Soc.*, 1955, 3555 (*ir*)
Tosi, L. *et al, Inorg. Chem.*, 1964, **3**, 150 (*ir*)
Tullberg, A. *et al, Acta Chem. Scand., Ser. A*, 1974, **28**, 340 (*struct*)
James, A.D. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1273 (*kinetics*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1658 (*Na salt*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, 1976, 130 (*rev, bibl*)
Johnson, C.R. *et al, Inorg. Chem.*, 1984, **23**, 2754 (*uv*)

IC-004671

$C_5H_3GeMnO_5$

Pentacarbonylgermylmanganese

[25069-08-3]

$H_3GeMn(CO)_5$

M 270.6
Synth. from H_3GeBr and $Na[Mn(CO)_5]$ in THF. Air-sensitive volatile white solid. Mp 23.8°. Ir ν_{CO} 2110s, 2020sh, 1980vs, 1960sh cm^{-1} (solid).

George, R.D. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1505 (*synth, ir, raman, pmr, ms*)
Inorg. Synth., 1974, **15**, 174 (*synth*)
Ebsworth, E.A.V., *Kem. Kozl.*, 1974, **42**, 1; *CA*, 1975, **82**, 9776 (*pe*)
Rankin, D.W. *et al, J. Organomet. Chem.*, 1975, **85**, 225 (*struct*)
Foster, S.P. *et al, J. Organomet. Chem.*, 1983, **247**, 21 (*pmr, ir*)

IC-004672

$C_5H_3MnO_5Si$

Pentacarbonylsilylmanganese, 9CI

[15770-61-3]

$H_3SiMn(CO)_5$

M 226.0
Synth. from SiH_3I and $Na[Mn(CO)_5]$. Air- and thermally-sensitive colourless solid. Mp 25.5°. Bp 134° (extrap.). Useful for synth. of Mn—Li films. Ir ν_{CO} 2096m, 2044w, 2010vs, 2006vs cm^{-1} (cyclohexane). Dec. at 118°.
▷ Shock-sensitive.

Bis-Py complex: [19697-64-4].
$C_{15}H_{18}MnN_2O_5Si$ M 389.3
Bright-yellow solid.

Aylett, B.J. *et al, J. Chem. Soc. A*, 1969, 1916 (*synth, ir, uv, pmr, raman, ms*)
Ebsworth, E.A.V., *Kem. Kozl.*, 1974, **42**, 1; *CA*, **82**, 9776 (*pe*)
Rankin, D.W. *et al, J. Organomet. Chem.*, 1975, **85**, 225 (*struct*)
Aylett, B.J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2058 (*thermal dec*)
Foster, S.P. *et al, J. Organomet. Chem.*, 1983, **247**, 21 (*pmr*)

IC-004673

$C_5H_3MnO_5Sn$

Pentacarbonylstannylmanganese

[71500-59-9]

$H_3SnMn(CO)_5$

M 316.7
Synth. from $HMn(CO)_5$ and SnH_4. Thermally unstable pale-yellow liq. Contaminated with Pentacarbonylhydromanganese, IC-004651.

Foster, S.P. *et al, J. Organomet. Chem.*, 1983, **247**, 21 (*synth, ir, pmr, ms*)

IC-004674

$C_5H_3MoO_5P$

Pentacarbonyl(phosphine)molybdenum

[23807-47-8]

$Mo(CO)_5PH_3$

M 269.9
Synth. by irradiation of $Mo(CO)_6$ in presence of PH_3. Almost colourless cryst. Mp 112° dec. Ir ν_{CO} 2081, 1986, 1956, 1925 cm^{-1} (hexane).

Fischer, E.O. *et al, Chem. Ber.*, 1969, **102**, 2547 (*synth, ir, pmr*)
Moser, E. *et al, J. Organomet. Chem.*, 1969, **19**, 377 (*pmr, P-31 nmr*)
Black, J.D. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2908 (*photol*)
Jeanne, C. *et al, Spectrochim. Acta, Part A*, 1975, **31**, 819 (*ir, raman*)

IC-004675

$C_5H_3N_4O_2Tc^{2\ominus}$

Tetrakis(cyano-*C*)methoxyoxotechnetate(2−), 10CI

Tetracyanomethoxyoxotechnetate(V)(*2*−)

$[TcO(OMe)(CN)_4]^{2\ominus}$

M 250.0 (ion)
trans-Octahedral geometry. Synth. from $TcOCl_4^{\ominus}$ and KCN in MeOH.

Di-K salt: Lavender-coloured solid.

Trop, H.S. *et al, Inorg. Chem.*, 1980, **19**, 1993 (*synth*)

$C_5H_5O_5PW$ IC-004676

Pentacarbonyl(phosphine)tungsten

[23807-48-9]

$W(CO)_5PH_3$

M 357.8

Synth. by irradiation of $W(CO)_6$ in presence of PH_3. Colourless cryst. (EtOH). Mp 136°. Ir ν_{CO} 2083, 1984, 1953, 1921 cm^{-1} (hexane).

Fischer, E.O. *et al, Chem. Ber.*, 1969, **102**, 2547 (*synth, ir, pmr, ms*)
Moser, E. *et al, J. Organomet. Chem.*, 1969, **19**, 377 (*pmr, P-31 nmr*)
Jeanise, C. *et al, Spectrochim. Acta, Part A*, 1975, **31**, 819 (*ir, raman*)
Dahlgreen, R.M. *et al, Inorg. Chem.*, 1977, **16**, 3154 (*synth, ir, pmr*)
Biel, F. *et al, J. Organomet. Chem.*, 1987, **328**, 349 (*synth, P-31 nmr, alkylation*)

$C_5H_4CrN_2O_5$ IC-004677

Pentacarbonyl(hydrazine-*N*)chromium, 9CI

[30092-08-1]

$(OC)_5CrNH_2NH_2$ (C_{4v})

M 224.0

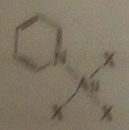
Yellow cryst. Mp 120–128°.

Sellmann, D., *Z. Naturforsch., B*, 1970, **25**, 890 (*synth*)
Sellmann, D. *et al, J. Organomet. Chem.*, 1976, **111**, 303 (*synth, props, ir, nmr*)

$C_5H_2AuBr_3N$ IC-004678

Tribromo(pyridine)gold(*III*), 10CI

[21524-04-9]



X = Br

M 515.7

Proposed four coordinate, planar struct. Deep red cryst. ($CHCl_3$). Insol. H_2O; v. spar. sol. Et_2O; sol. $CHCl_3$, Py. Evolves Py and dec. at ~150° without melting.

Gibson, C.S. *et al, J. Chem. Soc.*, 1931, 2497 (*synth, props*)
Brown, D.H. *et al, Inorg. Chim. Acta*, 1979, **32**, 137 (*synth, uv*)

$C_5H_2AuCl_3N$ IC-004679

Trichloro(pyridine)gold(*III*), 10CI

[14911-91-4]

As Tribromo(pyridine)gold(*III*), IC-004678 with

X = Cl

M 382.4

Yellow cryst. (CH_2Cl_2).

Belli Dell'Amico, D. *et al, Gazz. Chim. Ital.*, 1973, **103**, 1099; 1978, **108**, 627 (*synth*)
McKeller, A. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 767 (*pe*)

$C_5H_5BF_3N$ IC-004680

Trifluoro(pyridine)boron, 10CI

Pyridine compd. with trifluoroborane (1:1), 9CI. Pyridine compd. with boron fluoride (BF_3) (1:1), 8CI. Trifluoroborane pyridine

[407-76-1]

$F_3B{\leftarrow}Py$

M 146.9

Crosslinking agent for epoxy resins. White cryst. with very faint pyridine odour. Sol. C_6H_6, Py, hot EtOH; insol. Et_2O. Mp 45°, Mp 47-48°. Subl.$_{0.15}$ 100°, Bp 300°.

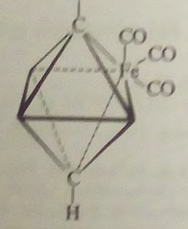
Van der Meulen, *et al, J. Am. Chem. Soc.*, 1932, **54**, 4404 (*synth*)
Luther, H. *et al, J. Prakt. Chem.*, 1958, **5**, 242 (*synth, ir, raman*)
Gates, P.N. *et al, Spectrochim. Acta*, 1965, **21**, 1445 (*synth, pmr, B-11 nmr*)
Perkampus, H.H. *et al, Ber. Bunsenges. Phys. Chem.*, 1967, **71**, 439 (*nmr*)
Hensen, K. *et al, Theor. Chim. Acta*, 1968, **12**, 206 (*uv*)
Taillandier, M. *et al, Spectrochim. Acta, Part A*, 1969, **25**, 1807 (*ir*)
Hensen, K. *et al, Chem. Ber.*, 1970, **103**, 2091 (*uv*)
Barber, M. *et al, J. Chem. Soc., Faraday Trans. 2*, 1973, **69**, 551 (*pe*)
Fraticello, A. *et al, J. Chem. Soc., Perkin Trans. 2*, 1983, 475 (*cmr, F-19 nmr*)
Töpsl, K.-H. *et al, Acta Crystallogr., Sect. C*, 1984, **40**, 828 (*cryst struct*)

$C_5H_5B_5FeO_3$ IC-004681

Tricarbonyl[η^4-pentahydrodicarbapentaborato(2−)]iron, 10CI

(1,2,4-$C_2B_3H_5$)tricarbonyliron

[53363-10-3]



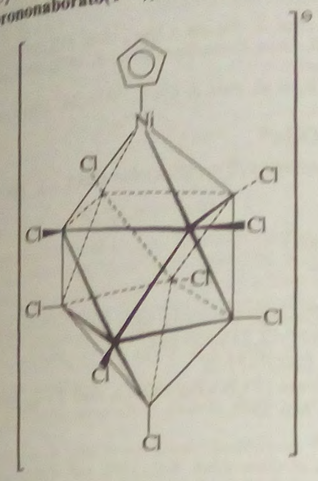
M 201.3

closo-borane. Orange liq. (by vacuum fractionation). Sol. CCl_4.

Miller, V.R. *et al, J. Am. Chem. Soc.*, 1974, **96**, 3090 (*synth, ir, B-11 nmr, pmr, ms*)
Armstrong, D.A. *et al, Inorg. Chim. Acta*, 1977, **21**, 55 (*theory*)
Ulman, J.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 456 (*pe*)

$C_5H_5B_5Cl_5Ni^{\ominus}$ IC-004682

(η^5-2,4-Cyclopentadien-1-yl)[η^5-nonachlorononaborato(1−)]nickelate(1−), 10CI



M 540.1 (ion)

closo-

Me_4N salt: [67635-30-7].
Yellow solid (aq. EtOH). Solns. unstable in sunlight.

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1978, **100**, 3758 (*synth, pmr, B-11 nmr, electrochem, uv-vis*)

$C_5H_5Cdl_2NO$ IC-004683

Diiodo(pyridine 1-oxide-*O*)cadmium(*II*), 9CI

(Pyridine 1-oxide)cadmium diiodide. Cadmium(II) iodide pyridine-1-oxide

[27838-05-7]

$(Py\text{-}O)CdI_2$

M 461.3

Polymeric chain struct. Cryst. (EtOH).

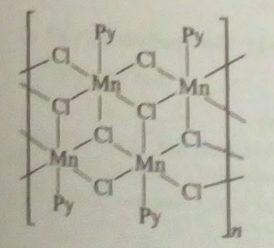
Ahuja, I.S. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 2665 (*synth, ir*)
Sawitzki, G. *et al, Chem. Ber.*, 1974, **107**, 3266 (*cryst struct*)

$C_5H_5Cl_2MnN$ IC-004684

Dichloro(pyridine)manganese(*II*), 10CI

Manganese(II) chloride pyridine

[72634-36-7]



M 204.9

Polymeric double-chain struct. with octahedral Mn. Synth. by thermal dec. of $MnCl_2Py_2$. Bromide and iodide also known. White solid; thermally unstable. Py lost at 255 and 315°. Insol. non-destructive solvs. Ir ν_{MnCl} 262-199; ν_{MnN} 160, 128, 118 cm^{-1}.

Allan, J.R. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1865 (*ir, uv*)
Murguiova, I.G. *et al, J. Therm. Anal.*, 1969, **1**, 97 (*thermal dec*)
Lipsey, G. *et al, J. Therm. Anal.*, 1970, **2**, 25 (*synth*)

Goldstein, M. *et al, Inorg. Chim. Acta*, 1979, **37**, 71 (*synth, ir, uv, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, D3, 102 (*rev, bibl*)

$C_5H_5Cl_2NNi$ IC-004685

Dichloro(pyridine)nickel(*II*), 8CI

Nickel(II) chloride pyridine

[14099-23-1]

$[NiCl_2(Py)]_n$

M 208.6

Polymeric structure with octahedral Ni. Also found as bromide and with picolines. Formed by thermal dec. of Dichlorobis(pyridine)nickel(*II*), IC-006796 or Dichlorotetrakis(pyridine)nickel(*II*), IC-010474. Yellow solid. Paramagnetic.

[28108-17-0]

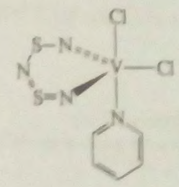
Nelson, S.M. *et al, J. Chem. Soc.*, 1965, 3276 (*synth, uv-vis, magnetism*)
Manolescu, D. *et al, Rev. Roum. Chim.*, 1969, **14**, 999 (*xrd*)
Goldstein, M. *et al, Inorg. Chim. Acta*, 1979, **37**, 71 (*ir, raman*)

$C_5H_5Cl_2N_4S_2V$ IC-004686

[(Aminothio)sulfur diimidato(3−)-$N^1,N^{2'}$] dichloro(pyridine)vanadium(*V*), 11CI

Dichloro(pyridine)cyclo-dithiatriazenovanadium(V)

[101332-56-3]



M 307.1

Trigonal bipyramid. Synth. from $VCl_3(N_3S_3)Py_2$ and $VCl_2(N_3S_3)$ in CH_2Cl_2. Black-brown solid. Sol. toluene. A bis(pyridine) adduct is also known.

Christophersen, R. *et al, Z. Naturforsch., B*, 1985, **40**, 1631 (*synth, cryst struct, ir, V-51 nmr*)

$C_5H_5Cl_3CoN^{\ominus}$ IC-004687

Trichloro(pyridine)cobaltate(*II*)(1−), 8CI

$[CoCl_3(Py)]^{\ominus}$

M 244.3 (ion)

Spectroscopic and magnetic data suggest a pseudo-tetrahedral struct. Paramagnetic.

Et_4N salt: [20045-54-9].
Sol. $MeNO_2$.

Brown, D.H. *et al, J. Chem. Soc. A*, 1968, 2146 (*synth, ir, uv, magnetism*)

$C_5H_5Cl_3MnN$ IC-004688

Trichloro(pyridine)manganese(*III*)

Manganese(III) chloride pyridine

$MnCl_3Py$

M 240.3

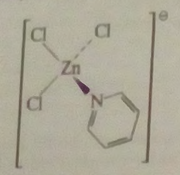
Structure unknown. See also Trichlorotris(pyridine) manganese(*III*), IC-008940. Synth. from components in Et_2O. Dark green leaflets, stable only below −10°.

Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **349**, 45 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 106 (*rev, bibl*)

IC-004689

$C_5H_5Cl_3NZn^{\ominus}$

Trichloro(pyridine)zincate(1 −)



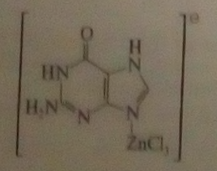
M 250.8 (ion)
Approx. tetrahedral Zn.
Et_4N salt: [20045-55-0].
Solid. Insol. Et_2O, EtOH, cyclohexane.
Pyridinium salt, Py complex: [72954-34-8]. *Pyridine, pyridinium trichloro(pyridine)zincate*
Cryst. Intra molecular H-bonds hold pairs of Py molecules together.

Bradbury, J. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2701 (*ir, Et_4N salt*)
Brown, D.H. *et al*, *J. Chem. Soc. A*, 1968, 2146 (*synth, ir, Et_4N salt*)
Mohapatra, B.K. *et al*, *J. Inst. Chem. (India)*, 1970, **42**, 199 (*synth, PyH salt*)
Villarreal-Salinas, B.E. *et al*, *J. Cryst. Mol. Struct.*, 1978, **8**, 217 (*struct, PyH salt*)
Kistenmacher, T.J., *J. Cryst. Mol. Struct.*, 1979, **9**, 325 (*struct, Py_2H salt*)

IC-004690

$C_5H_4Cl_3N_3OZn^{\ominus}$

Trichloro(guanine)zincate(1 −)
(2-Amino-1,7-dihydro-6H-purin-6-one-N^9) trichlorozincate(1 −), 9Cl



Solid state struct.

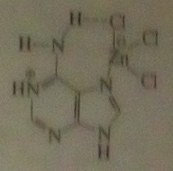
M 322.8 (ion)
H compd.: [31116-43-5]. *(Guaninium)trichlorozinc* $C_5H_4Cl_3N_3OZn$ M 323.8
Cryst. (aq. acid). Sol. DMSO.

Srinivasan, L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 1668 (*synth, cryst struct*)
Walker, W. *et al*, *Aust. J. Chem.*, 1973, **26**, 2391 (*synth, pmr*)

IC-004691

$C_5H_4Cl_3N_5Zn^{\ominus}$

(Adenine)trichlorozincate(1 −)
Trichloro(9H-purine-6-amine-N^3)zincate(1 −), 9Cl



H compd.

M 306.8 (ion)
Monomeric, tetrahedral Zn.
H compd.: [30974-58-4].
Cryst. (H_2O). Sol. DMSO.

Weitzel, G. *et al*, *Z. Physiol. Chem.*, 1958, **313**, 212 (*synth*)
Taylor, M.R., *Acta Crystallogr., Sect. B*, 1973, **29**, 884 (*synth, cryst struct*)
Walker, W.R. *et al*, *Aust. J. Chem.*, 1973, **26**, 2391 (*synth, pmr*)

IC-004692

$C_5H_5Cl_4N_2ORe^{\ominus}$

Tetrachloronitrosyl(pyridine)rhenate(1 −), 10Cl

$[Re(NO)Cl_4Py]^{\ominus}$

M 437.1 (ion)
Octahedral.

trans-form
Linear Re-N-O grouping with Re—N 178.9, N—O 117.1, Re—Cl 235-238 pm.

Et_4N salt: [65877-77-2].
Synth. from $(Et_4N)_2Re(NO)Cl_5$ and Py in EtOH or MeCN. Mp 214°.

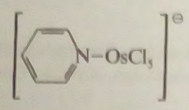
[60542-96-3]

Ciani, G. *et al*, *Gazz. Chim. Ital.*, 1977, **107**, 429 (*synth, ir, props*)
Ciani, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 798 (*cryst struct*)

IC-004693

$C_5H_5Cl_5NOs^{\ominus}$

Pentachloro(pyridine)osmate(*IV*)(1 −)
[63985-27-3]



M 446.5 (ion)
Synth. by photolysis at $[OsCl_6]^{2\ominus}$ in Py. Stable in acidic soln.

Cs salt: [75441-29-1].
Tetrabutylammonium salt: [63985-28-4].
Pale yellow solid (hexane/CH_2Cl_2). Insol. H_2O, C_6H_6. Na, K, $PPh_4^{\oplus}$ salts also known.

Hasenpusch, W. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **432**, 107 (*synth*)
Preetz, W. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **445**, 5 (*synth, props*)
Schukla, A.K. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **468**, 39 (*synth, uv, ir*)

IC-004694

$C_5H_5Cl_5NPd^{\ominus}$

Pentachloro(pyridine)palladate(*IV*)(1 −)

$[PdCl_5(Py)]^{\ominus}$

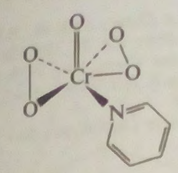
M 362.7 (ion)
Tetrabutylammonium salt: [83971-01-1].
Moisture-sensitive orange solid. Sol. CH_2Cl_2.

Gulliver, D.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1896 (*synth, ir, uv-vis*)

IC-004695

$C_5H_5CrNO_5$

Oxodiperoxy(pyridine)chromium(*VI*), 11Cl, 9Cl
(Oxodiperoxopyridinechromium(VI)
[33361-75-0]



M 211.0
Pentagonal pyramidal struct. Interatomic distances: Cr=O 157.6, Cr—N 204.7pm. Relat. compds. with ligands replacing Py also known. Synth. by action of H_2O_2 on acidified dichromate followed by extraction into Py/Et_2O. Oxidant for org. synth. Deep blue cryst. Sol. CH_2Cl_2, $CHCl_3$, C_6H_6, insol. H_2O. Mp 102° dec.
▷ Dry solid is explosive.

Pedersen, B.F. *et al*, *Acta Chem. Scand.*, 1963, **17**, 557 (*cryst struct*)
Connor, J.A. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1964, **6**, 279 (*rev*)
Stomberg, R., *Ark. Kemi.*, 1964, **22**, 29 (*cryst struct*)
Armstrong, R. *et al*, *Aust. J. Chem.*, 1968, **21**, 897.
Fleet, G.W.J. *et al*, *Tetrahedron Lett.*, 1977, **42**, 3749 (*use*)
Hester, R.E. *et al*, *J. Raman Spectrosc.*, 1981, **11**, 39 (*raman*)
Ruggero, C. *et al*, *J. Mol. Catal.*, 1985, **32**, 251 (*O-17 nmr*)
Firouzabadi, H. *et al*, *Tetrahedron*, 1986, **42**, 719 (*use*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 945 (*rev*)

IC-004696

$C_5H_5I_3NNi^{\ominus}$

Triiodo(pyridine)nickelate(*II*)(1 −)

$PyNiI_3^{\ominus}$

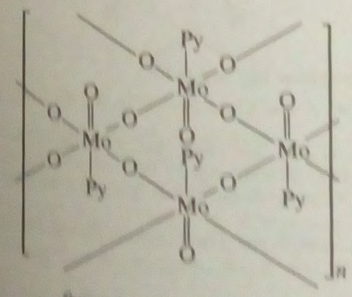
M 518.5 (ion)
Tetrahedral struct. Model for C_{3v} local symmetry for $Ni^{2\oplus}$.
N-Propylpyridinium salt: [21489-09-8].
$C_{13}H_{17}I_3N_2Ni$ M 640.6
Moisture-sensitive, dark green solid. Unstable in soln.
μ_{eff} = 3.72 μ_B (291K).

Brown, D.H. *et al*, *J. Chem. Soc. A*, 1968, 2146 (*synth, far-ir, electronic spect, magnetism*)

IC-004697

$C_5H_5MoNO_3$

Trioxo(pyridine)molybdenum(*VI*), 10Cl
Pyridinemolybdenum trioxide. Molybdenum(VI) *oxide pyridine*
[78671-70-2]



M 223.0

Fragment of layer

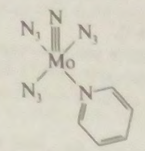
Polymeric layer struct. All O atoms in horizontal plane are shared. Synth. from excess Py heated with MoO_3 under strictly anhydrous conditions. Has potential catalytic and sorptive props. Microcryst.

Johnson, J.W. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 5246 (*cryst struct*)
Johnson, J.W. *et al*, *Rev. Chim. Minér.*, 1982, **19**, 420 (*synth, ir, tga, struct*)

IC-004698

$C_5H_5MoN_{11}$

Triazidonitrido(pyridine)molybdenum(*VI*), 10Cl
Tris(azido)nitridopyridinemolybdenum(VI)
[78505-55-2]



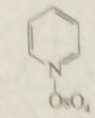
M 315.1
Red cryst. Hydrol. rapidly in moist air.
▷ Explosive.

Schweda, E. *et al*, *Z. Naturforsch., B*, 1981, **36**, 662 (*cryst struct, synth*)

IC-004699

$C_5H_5NO_4Os$

Tetraoxopyridineosmium(*VIII*)
Osmium tetroxide pyridine complex
[39051-33-7]



M 333.2
Synth. from excess Py and OsO_4 in cyclohexane. Bright yellow cryst. Sol. CCl_4, $CHCl_3$, insol. H_2O. Ir $\nu_{Os=O}$ 926w, 915s, 908s, 885m, 360m, 298w cm^{-1}; Raman $\nu_{Os=x}$ *ca.* 200 cm^{-1}.

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1449 (*synth, ir, raman*)
Nikol'skii, A.B., *Zh. Neorg. Khim.*, 1974, **19**, 1889; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 1031 (*synth, ir, raman*)
Lin'ko, I.V. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 1520 (*pe*)

IC-004700

$C_5H_5O_{40}SiTiV_3W_9^{4\ominus}$

(η^5-2,4-Cyclopentadien-1-yl)[μ_{13}-[orthosilicato(4 −)-*O:O:O:O :O :O :O :O :O :O :O :O*]]tetra-μ-oxotri-μ_3-oxo(tetradeca-μ-oxononaoxononatungstate)(tri-μ-oxotrioxotrivanadate)titanate(4 −), 11Cl

$[(C_5H_5)TiSiW_9V_3O_{40}]^{4\ominus}$

M 2588.5 (ion)
Structure not certain.
Tetrakis-tetrabutylammonium salt: [92786-65-7].
$C_{68}H_{149}N_4O_{40}SiTiV_3W_9$ M 3558.3
Model oxide, soluble vanadium(*V*) heteropolyanion.
Dark-orange cryst. ($CHCl_3$/MeCN). Insol. MeOH, EtOH.

Finke, R.G. *et al*, *Organometallics*, 1988, **8**, 175 (*synth, ir, Si-29 nmr, H-1/51 nmr, ms*)

IC-004701

$C_5H_6B_2O_5Re^{\ominus}$

Bis(borane)pentacarbonylrhenate(1−), 8CI

$[Re(CO)_5(BH_3)_2]^{\ominus}$

M 353.9 (ion)
Struct. not established. Salts are drying agents, and selective reducing agents.

Na salt: [19632-39-4].
$C_5H_6B_2NaO_5Re$ M 376.9
Air and moisture sensitive solid (Et_2O). Sol. ethers, THF.

Cs salt: [19584-34-0].
Air and moisture sensitive solid ($2Et_2O$). Sol. ethers, THF.

Et_4N salt: [19584-35-1].
Moisture-air sensitive yellow-orange cryst. (THF/Et_2O).

Tetrabutyiphosphonium salt: [19632-40-7].
Moisture and air sensitive red-orange cryst. (THF/Et_2O).

Parshall, G.W., *J. Am. Chem. Soc.*, 1964, **86**, 361 (*synth, ir, pmr, ms*)
U.S. Pat., 3 330, (1967); *CA*, **67**, 92434d (*synth, ir, props*)

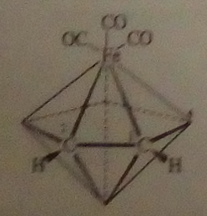
IC-004702

$C_5H_6B_4FeO_3$

Tricarbonyl[(2,3,4,5,6-η)-hexahydro-2,3-dicarbahexaborato(2−)]iron, 9CI

1,2,3-Tricarbonyliron-$C_2B_4H_6$-(π-2,3-$C_2B_4H_6$)tricarbonyliron

[51177-52-7]



M 213.1
closo- Deep yellow-orange liq.

Grimes, R.N., *J. Am. Chem. Soc.*, 1971, **93**, 261 (*synth, ms, nmr, pmr, ir*)
Sneddon, L.G. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6623 (*synth, ms, pmr, nmr, ir*)

IC-004703

$C_5H_6B_4FeO_3$

Tricarbonyl[(2,3,4,5,6-η)-hexahydro-2,4-dicarbahexaborato(2−)]iron

1,2,4-(Tricarbonyliron)-$C_2B_4H_6$ (π-2,3-$C_2B_4H_6$) tricarbonyliron

M 213.1
Yellow-orange liq.

Sneddon, L.G. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6623 (*synth, nmr, pmr, ir*)

IC-004704

$C_5H_6Cl_4N_2Ti$

catena-Tetrachloro(μ-pentane-1,5-dinitrile)titanium(IV)

Tetrachloro(pentanedinitrile-N)titanium(IV), 10CI
Tetrachloro(glutaronitrile)titanium, 8CI
Titanium(IV) chloride pentanedinitrile
catena-μ-Pentane-1,5-dinitrile-tetrachlorotitanium(IV)

[14276-47-2]

$[N{\equiv}C(CH_2)_3C{\equiv}N{\rightarrow}TiCl_4]_n$

M 280.8

Octahedral polymer. N atoms are *cis*. Synth. from $TiCl_4$ and ligand in CH_2Cl_2. Varying the proportions yields 2:1, 1:1 and 1:2 complexes. Catalyses olefin trimerisation. Yellow solid. Mp 215° dec.

[12548-44-6]

Jain, S.C. *et al*, *Can. J. Chem.*, 1963, **41**, 2130 (*synth, ir*)
Fr. Pat., 2 004 108, (1968); *CA*, **72**, 132165d (*use*)
Kubota, M. *et al*, *J. Am. Chem. Soc.*, 1976, **88**, 2451 (*ir, conformn*)
Ling-Kang, L. *et al*, *Bull. Inst. Chem. Acad. Sin.*, 1985, **32**, 45 (*synth, cryst struct*)
Ling-Kang, L. *et al*, *Acta Crystallogr., Sect. C*, 1986, **42**, 1986 (*cryst struct*)

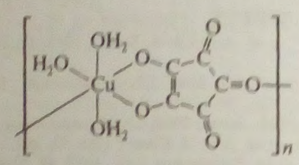
IC-004705

$C_5H_6CuO_8$

Triaqua[4,5-dihydroxy-4-cyclopentene-1,2,3-trionato(2−)-O^4,O^5]copper(*II*), 9CI

Copper(II) *croconate*. *[4,5-Dihydroxy-4-cyclopentene-1,2,3-trionato(2−)]triaquocopper*

[38722-38-2]



M 257.6
The D_{5h} symmetry of the dianion is essentially retained. Approx. octahedral at Cu. Reddish brown cryst. Insol. H_2O, Me_2CO, Et_2O.

West, R. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 2586 (*synth, magnetism, ir*)
Glick, M.D. *et al*, *Inorg. Chem.*, 1964, **3**, 1712 (*cryst struct*)
Jeter, D.Y. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 2767 (*magnetism, synth*)
Bottei, R.S. *et al*, *J. Therm. Anal.*, 1979, **16**, 389 (*thermal props*)

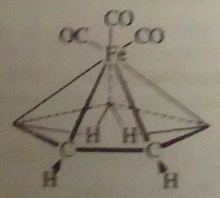
IC-004706

$C_5H_7B_3FeO_3$

Tricarbonyl[(1,2,3,4,5-η)-heptahydro-1,2-dicarbapentaborato(2−)]iron, 10CI

Dicarbacyclopentaboranyliron tricarbonyl. *Tricarbonyliron-(2,3-$C_2B_3H_7$)*

[33362-89-9]



M 209.3
nido- Pale-yellow liq. Mp 0-15°.

Grimes, R.N., *J. Am. Chem. Soc.*, 1971, **93**, 261 (*synth, pmr, ms, ir*)
Franz, D.A. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 412 (*synth*)
Brennan, J.P. *et al*, *Inorg. Chem.*, 1973, **12**, 2266 (*struct*)
Sneddon, L.G. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6623 (*synth, nmr, ir*)
Ulman, J.A. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 456 (*pr*)

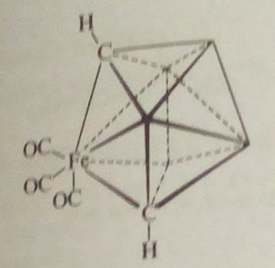
IC-004707

$C_5H_7B_3FeO_3$

Tricarbonyl[(3,4,5,6,7-η)-heptahydro-3,5-dicarbaheptaborato(2−)]iron, 9CI

4,1,8-(Tricarbonyliron)-$C_2B_5H_7$

[51203-46-4]



M 225.0
Orange.

Sneddon, L.G. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 6623 (*synth, nmr, pmr, ir*)

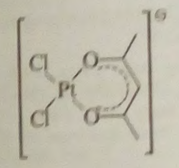
IC-004708

$C_5H_7Cl_2O_2Pt^{\ominus}$

Dichloro(2,4-pentanedionato)platinate(*II*)(1−), 8CI

(Acetylacetonato)dichloroplatinate(II)

[76647-71-7]



M 365.0 (ion)
One of many products from $PtCl_4^{2\ominus}$ + 2,4-pentanedione; acac here is bonded through 2 oxygens.

K salt: [15246-03-4].
$C_5H_7Cl_2KO_2Pt$ M 404.1
Yellow-orange plates. Sol. H_2O.

Lewis, J. *et al*, *J. Chem. Soc.*, 1965, 6740 (*pmr*)
Bennke, G.T. *et al*, *Inorg. Chem.*, 1967, **6**, 433 (*synth, ir*)

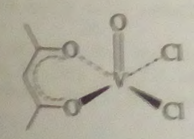
IC-004709

$C_5H_7Cl_2O_3V$

Dichlorooxo(2,4-pentanedionato-O,O')vanadium(*V*), 11CI

(Acetylacetonato)dichlorooxovanadium(V). *Oxodichloro(2,4-pentanedionato)vanadium*(V)

[14709-83-2]



M 226.9
Pale yellow sq. pyramidal. Synth. from $VOCl_3$ + 2,4-pentanedione in C_6H_6. Polym. catalyst. Red, hygroscopic solid. Mp 200° dec. Ir $\nu_{V=O}$ 965 cm^{-1}.

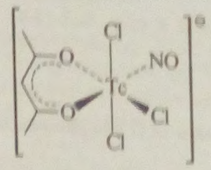
Japan. Pat., 7 307 513, (1973); *CA*, **80**, 27706y (*use*)
Japan. Pat., 78 41 196, (1978); *CA*, **90**, 55519q (*use*)
Quintero Lopez, A. *et al*, *An. Quim., Ser. B*, 1981, **77**, 305 (*synth, ir*)
Joseph, K. *et al*, *Indian J. Chem., Sect. A*, 1983, **22**, 159 (*synth, ir*)

IC-004710

$C_5H_7Cl_3NO_3Tc^{\ominus}$

Trichloronitrosyl(2,4-pentanedionato-O,O')technetate(1−)

(Acetylacetonato)trichloro(nitrosyl)technetate(1−)



M 334.3 (ion)
Formally a technetium(*II*) complex. Synth. from $TcO_4^{\ominus}$ by NH_2OH reduction in HCl followed by reaction with acacH.

Ph_4As salt: [116155-34-1].
Red solid (MeOH aq.). Sol. CH_2Cl_2.

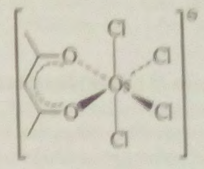
Brown, D.S. *et al*, *Inorg. Chim. Acta*, 1988, **150**, 193 (*synth, cryst struct, ir, ms, esr*)

IC-004711

$C_5H_7Cl_4O_2Os^{\ominus}$

Tetrachloro(2,4-pentanedionato-O,O')osmate(*IV*)(1−)

(Acetylacetonato)tetrachloroosmate(IV)(1−)



M 431.1 (ion)
Approx. octahedral.

Cs salt: [60173-43-5].
Synth. from $Cs_2[OsCl_6]$ and acetylacetone. Ir ν_{Os-Cl} 350vs, 334m, 324vs cm^{-1}.

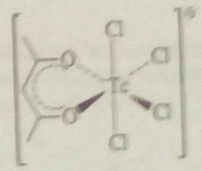
Schaetzel, G. *et al*, *Z. Naturforsch., B*, 1976, **31**, 749 (*synth, ms, ir*)

IC-004712

$C_5H_7Cl_4O_2Tc^{\ominus}$

Tetrachloro(2,4-pentanedionato-O,O')technetate(*IV*)(1−), 10CI

(Acetylacetonato)tetrachlorotechnetate(IV)(1−)



M 339.8 (ion)
Approx. octahedral anion. Synth. from $[TcCl_6]^{2\ominus}$ + ligand.

Ph_4P salt: [71128-01-3].
Red prisms. Sol. CH_2Cl_2, spar. sol. Me_2CO, C_6H_6, EtOH; insol. ethers, hydrocarbons. Mp 225° dec.

Mazzi, U. *et al*, *Transition Met. Chem.*, 1979, **4**, 151 (*synth, ir, ac. props, magnetism*)

IC-004713

$C_5H_7F_4MnNO$

Aquatetrafluoro(pyridine)manganese(*IV*)

$MnF_4(OH_2)(Py)$

M 228.0

Struct. not known. Synth. from $KMnO_4$, Py and 48% HF. Useful for the synth. of $[MnF_4]^{\ominus}$ anions. Brown needles; stable at r.t., does not attack glass in absence of H_2O but has a faint smell of Py. Sol. 48% HF. $\mu_{eff} = 3.98\mu_B$ (302K).

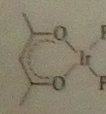
Chaudhuri, M.K. *et al, J. Inorg. Nucl. Chem.*, 1981, **43**, 85 (*synth, ir, magnetism*)

$C_5H_4F_4IrO_2P_2$ IC-004714

(2,4-Pentanedionato-*O,O'*)bis(phosphorous trifluoride) iridium(*I*), 8Cl

(2,4-Pentanedionato)bis(trifluorophosphine)iridium(I). *(Acetylacetonato)bis(trifluorophosphine)iridium*(I)

[34228-56-3]



M 467.2

Square planar. Orange cryst. (pentane). Sol. pentane, C_5H_{12}.

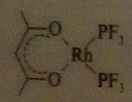
Bennett, M.A. *et al, Inorg. Chem.*, 1971, **10**, 2387 (*synth, ir, F-19 nmr*)

$C_5H_4F_6O_2P_2Rh$ IC-004715

(2,4-Pentanedionato-*O,O'*)bis(phosphorous trifluoride) rhodium, 8Cl

2,4-Pentanedionatobis(trifluorophosphine)rhodium(I). *Acetylacetonatobis(trifluorophosphine)rhodium*(I)

[34267-87-3]



M 377.9

Prob. square planar struct. Orange cryst. Sol. pentane. Mp 75-77°.

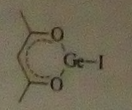
Bennett, M.A. *et al, Inorg. Chem.*, 1971, **10**, 2387 (*synth, ir, pmr, F-19 nmr*)

$C_5H_5GeIO_2$ IC-004716

Iodo(2,4-pentanedionato-*O,O'*)germanium, 9Cl

(Pentane-2,4-dionato)germanium(II) *iodide*

[59269-05-5]



M 298.6

A monomeric germylene deriv., containing 3-coord. Ge. Synth. from GeI_2 + Na(acac) in anhydrous THF. Extremely air- and moisture-sensitive bright yellow cryst. Mp 49-51°.

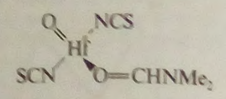
Rodgers, A. *et al, J. Chem. Soc., Chem. Commun.*, 1976, 52 (*synth*)
Stobart, S.R. *et al, J. Chem. Soc., Chem. Commun.*, 1979, 911 (*cryst struct*)

$C_5H_7HfN_3O_2S_2$ IC-004717

(*N,N*-Dimethylformamide-*O*)oxobis(thiocyanato-*N*) hafnium(*IV*), 11Cl

Oxobis(isothiocyanato)(N,N-dimethylformamide) hafnium(IV)

[88609-58-9]



M 383.7

Synth. from $HfOCl_2$ and KSCN in DMF.

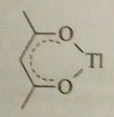
Kharitonova, Yu.Ya. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 1803 (*synth, ir, thermal anal*)

$C_5H_7O_2Tl$ IC-004718

(2,4-Pentanedionato)thallium(*I*)

(Acetylacetonato)thallium(I)

[14219-90-0]



M 303.4

Prepd. from Tl + 2,4-pentanedione in EtOH. White cryst. ($CHCl_3$). Mp 160-5°.

West, R. *et al, J. Inorg. Nucl. Chem.*, 1958, **5**, 295 (*synth, ir*)
Smith, J.A.S. *et al, J. Chem. Soc. A*, 1966, 1749 (*pmr*)
Wilkie, C.A. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 195 (*cmr*)
Nihoul, B. *et al, Adv. Mass Spectrom. A*, 1987, **7**, 605 (*ms*)

C_5H_8BN IC-004719

Trihydro(pyridine)boron, 10Cl

Borane pyridine. Pyridine compd. with borane(1:1), 9Cl, 8Cl

[110-51-0]

BH_3Py

M 92.9

Germicide, fungicide, and protozoicide, used in photographic colour development of reversal films. Reducing agent. Commercially available. Liq. Mp 10-11°. n_D^{20} 1.5315.

▷ Toxic, flammable. US3675000.

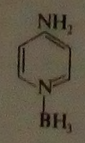
Brey, W.S. *et al, Adv. Chem. Ser.*, 1964, **42**, 100 (*nmr*)
Hoffmann, R., *J. Chem. Phys.*, 1964, **40**, 2474 (*struct*)
Hermanek, S. *et al, Collect. Czech. Chem. Commun.*, 1966, **31**, 1281 (*chromotog*)
Andrews, G.C., *Tetrahedron Lett.*, 1980, **21**, 697.
Schaefer, T. *et al, Can. J. Chem.*, 1981, **59**, 3026 (*struct*)
Pelter, A. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 1014.

$C_5H_9BN_2$ IC-004720

(4-Aminopyridine)trihydroboron

Borane 4-aminopyridine. Trihydro(4-pyridinamine-N¹)boron, 10Cl. 4-Pyridinamine compd. with borane(1:1), 9Cl

[59900-43-5]



M 107.9

Used in photographic developer solns.

Max, C.E. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1977, **7**, 509
U.S. Pat. 4 042 392, (1977); *CA*, **88**, 30399w.
Lelental, M. *et al, J. Photogr. Sci.*, 1978, **26**, 135 (*use*)

$C_5H_4CdN_2O_5$ IC-004721

Aqua[glutamato(2 –)]cadmium

$Cd(OH_2)[OOCCH_2CH_2CH(NH_2)COO]$

M 289.5

V. approx. octahedral Cd with extensive bridging of glutamate ligand.

x-form [50989-19-0]

Cryst. + $1H_2O$ (H_2O).

[55049-27-9, 62454-99-3]

Flook, R.J. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 753 (*cryst struct*)
Soylu, H. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1974, **140**, 281 (*synth, cryst struct*)
Flook, R.J. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 801 (*cryst struct, nd*)
Ashby, C.I.H. *et al, J. Am. Chem. Soc.*, 1980, **102**, 2990 (*synth, N-14 ngr*)

$C_5H_9NO_2PbS$ IC-004722

D-Penicillaminatolead(*II*)

[3-Mercapto-D-valinato(2 –)-N,O,S]lead

[53513-80-7]

$Pb[SC(CH_3)_2CH(NH_2)COO]$

M 354.3

The ligand is tridentate. Prepd. from a soln. of $Pb(NO_3)_2$ and D-penicillamine in H_2O. Formation of this complex is involved in the treatment of lead poisoning by D-penicillamine. Cryst.

[56093-08-4]

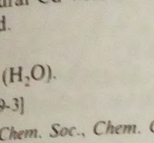
Sugiura, Y. *et al, Chem. Pharm. Bull.*, 1970, **18**, 693 (*stability const*)
Freeman, H.C. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 366 (*synth, cryst struct*)

$C_5H_9O_3P$ IC-004723

4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane, 9Cl

Methyl bicyclic phosphite. Trimethylolethane phosphite

[1449-91-8]



M 148.0

Ligand for metals of groups IB, VIB, VIIB, and VIII. Solid. Mp 94°. Subl.$_{0.02}$ 50°.

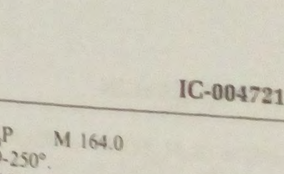
▷ V. toxic. TY7200000.

B, Ph_3CClO_4: *4-Methyl-4-triphenylmethyl-2,6,7-trioxa-1-phosphoniabicyclo[2.2.2]octane perchlorate*
$C_{24}H_{24}ClO_7P$ M 490.8
Cryst. (MeCN). Mp 198°.
B, Ph_3CBF_4: *4-Methyl-4-triphenylmethyl-2,6,7-trioxa-1-phosphoniabicyclo[2.2.2]octane tetrafluoroborate*
$C_{24}H_{24}BF_4O_3P$ M 478.2
Cryst. (Me_2CO). Mp 183°.
1-Oxide. [1449-89-4]. *Trimethylolethane phosphate. Methyl bicyclic phosphate*
$C_5H_9O_4P$ M 164.0
Mp 249-250°.
▷ Toxic. LD_{50} 32 mg/kg (mouse, ip). YK0711700.
1-Sulfide: [3196-56-3]. *Trimethylolethane thiophosphate. Methyl bicyclic thiophosphate*
$C_5H_9O_3PS$ M 180.1
Cryst. (1,2-dimethoxyethane). Mp 216-218°.
▷ Toxic. LD_{50} 34 mg/kg (mouse, ip). TE9450000.
1-Selenide: [67471-54-9]. *Trimethylol selenophosphate. Methyl bicyclic selenophosphate*
$C_5H_9O_3PSe$ M 227.0
Cryst. (toluene). Mp 246-248°.

Wadsworth, W.S. *et al, J. Am. Chem. Soc.*, 1962, **84**, 610.
Verkade, J.G. *et al, Inorg. Chem.*, 1965, **4**, 83 (*synth, pmr*)
Nimrod, D.M. *et al, J. Am. Chem. Soc.*, 1968, **90**, 2780 (*oxide, cryst struct*)
Keiter, R.L. *et al, Inorg. Chem.*, 1970, **9**, 404 (*complexes*)
Bellet, E.M. *et al, Science (Washington, D.C.)*, 1973, **182**, 1135 (*tox*)
Cowley, A.H. *et al, Inorg. Chem.*, 1977, **16**, 854; 1984, **23**, 3378 (*pe*)
Kroshefsky, R.D. *et al, Inorg. Chem.*, 1979, **18**, 469 (*selenide, synth, P-31 nmr*)
Voorhees, K.J. *et al, Org. Mass Spectrom.*, 1979, **14**, 459 (*ms*)
Kenttamaa, H. *et al, Org. Mass Spectrom.*, 1980, **15**, 520 (*derivs, ms*)
Fanni, T. *et al, J. Am. Chem. Soc.*, 1986, **108**, 6311 (*props*)
Eliel, E.L. *et al, J. Am. Chem. Soc.*, 1986, **108**, 6651 (*O-17 nmr*)

$C_5H_{10}B_3^{\ominus}$ IC-004724

2,3-Dimethyl-2,3,4-tricarbahexaborate(1 –)



M 102.5 (ion)

Proposed *nido*- struct. shown.

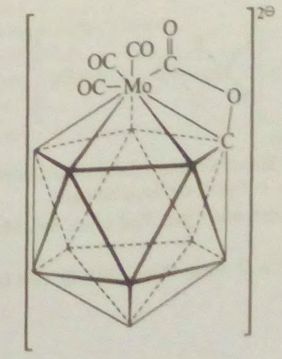
Na salt: Synth. from $Me_2C_2B_3H_5$ + NaH in mineral oil. V. moisture-sensitive solid. Sol. diglyme with dec.

Grimes, R.N. *et al, J. Am. Chem. Soc.*, 1969, **91**, 4010 (*synth, ir, B-11 nmr*)

$C_5H_{10}B_{10}MoO_5^{2\ominus}$ IC-004725

Tricarbonylcarboxy[decahydro-7-hydroxy-π-7-carbaundecaborato(1 –)]molybdate(2 –) lactone, 8Cl

[29386-89-8]



M 354.1 (ion)

May be converted to $(B_{10}H_{10}COH)Mo(CO)_4^{\ominus}$ by aq. acid in the absence of air.

Bis-tetrabutylammonium salt: Yellow cryst. Sol. MeCN.

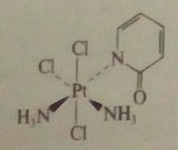
Wegner, P.A. *et al, J. Am. Chem. Soc.*, 1970, **92**, 3473 (*synth, ir, B-11 nmr, cryst struct*)

IC-004726

$C_5H_{10}Cl_2N_3OPt$

Diamminetrichloro(2(1*H*)-pyridinonato-*N*)platinum(*IV*), 11Cl

[86471-90-1]



M 429.5

Has *mer*-chlorides, *cis*-NH_3. Yellow cryst.

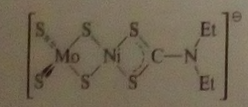
Hollis, L.S. *et al, Inorg. Chem.*, 1983, **22**, 2708.

IC-004727

$C_5H_{10}MoNNiS_6^{\ominus}$

Diethyldithiocarbamato[tetrathiomolybdato(*VI*)]nickelate(*II*)(1−)

[(Diethylcarbamodithioato-S,S′)nickelate(II)]di-μ-thioxodithioxomolybdate(IV)(1−), 10CI



M 431.1 (ion)

Struct. contains square planar Ni and tetrahedral Mo.

Synth. from Bis[tetrathiomolybdato(*VI*)]nickelate(*II*)(2−), IC-020818 + Bis(*N,N*-diethyldithiocarbamato)nickel(*II*), IC-007082.

Tetrapropylammonium salt: [77071-63-7].

Appearance not described. Sol. MeCN. Mp 149-150° (dec.).

Callahan, K.P. *et al, Inorg. Chem.*, 1981, **20**, 1941 (*synth, ir, uv, props*)

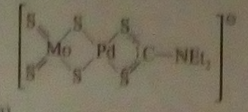
IC-004728

$C_5H_{10}MoNPdS_6^{\ominus}$

Diethyldithiocarbamato(tetrathiomolybdato)palladate(*II*)(1−)

(Diethyldithiocarbamatopalladate)di-μ-thioxodithioxomolybdate(1−), 11CI

[77079-68-6]



M 478.8 (ion)

Synth. from Bis(tetrathiomolybdato)palladate(*II*)(2−), IC-020826 + Pd(*II*) dithiocarbamate.

Tetrapropylammonium salt: Red cryst. Sol. MeCN. Mp 173-174°.

Callahan, K.P. *et al, Inorg. Chem.*, 1981, **20**, 1941 (*synth, ir, uv, elec cond*)

IC-004729

$C_5H_{10}NNaS_2$

Sodium diethyldithiocarbamate

Diethyldithiocarbamic acid, sodium salt, 8CI.
Diethylcarbamodithioic acid, sodium salt, 9CI. Ditiocarb sodium INN. Dithiocarb. Cupral. Imuthiol. DTC

[148-18-5]

$Na(S_2CNEt_2)$

M 171.2

Reagent for the extraction of metal cations. Antidote for acute metal poisoning. Component of copper electroless coating solns. Cryst. (EtOH). Sol. H_2O, EtOH.

▷ EZ6475000.

Trihydrate: [20624-25-3].
$C_5H_{16}NNaO_3S_2$ M 225.3
Commercially available. Orthorhombic cryst.
▷ EZ6550000.

Malissa, H. *et al, Talanta*, 1961, **8**, 841 (*struct*)
Evtushenko, N.P., *Ukr. Khim. Zh.* (*Russ. Ed.*), 1965, **31**, 618 (*ir*)
Tosi, L. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 53 (*raman*)
van Gaal, H.L.M. *et al, Inorg. Chem.*, 1979, **18**, 3251 (*cmr*)
Yu, J.C.M. *et al, Anal. Chem.*, 1984, **56**, 1689 (*uses*)
Mereiter, K. *et al, Inorg. Chim. Acta*, 1985, **98**, 71 (*trihydrate, struct, raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1206A (*haz, trihydrate*)

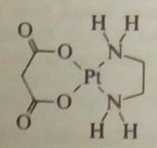
IC-004730

$C_5H_{10}N_2O_4Pt$

1,2-Ethanediamine[propanedioato(2−)-*O,O′*]platinum(*II*), 9CI

Ethylenediamine(malonato)platinum(II). *JM 40*

[41666-77-7]



M 357.2

Square planar struct. Has potential use as anticancer drug. Cryst.

▷ TP2505500.

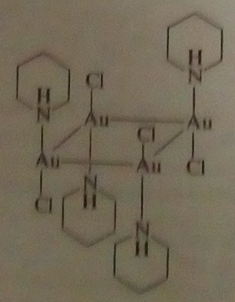
Cutbush, S.D. *et al, J. Inorg. Biochem.*, 1983, **18**, 213 (*cryst struct*)
Boven, E. *et al, Cancer Res.*, 1985, **45**, 86 (*use*)

IC-004731

$C_5H_{11}AuClN$

Chloro(piperidine)gold(*I*), 9CI

[62429-03-2]



tetramer

M 317.5

Weakly bound tetramer in solid state.

Tetramer: Tetrachlorotetrapiperidinetetragold
$C_{20}H_{44}Au_4Cl_4N_4$ M 1270.2

V. air-sensitive colourless cryst. (CH_2Cl_2/pet. ether); dec. readily to metallic gold. Mean Au—Au distance 330pm.

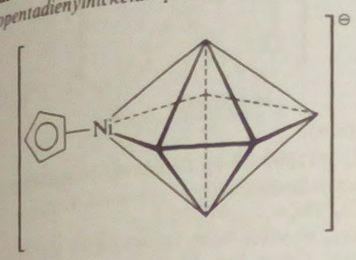
Guy, J.J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 8 (*synth, cryst struct*)

IC-004732

$C_5H_{11}B_6Ni^{\ominus}$

(η⁴-2,4-Cyclopentadien-1-yl)[η⁴-hexahydrohexaborato(2−)]nickelate(1−), 11Cl

η⁴-Cyclopentadienylnickelaheptaborate(1−)



M 194.6 (ion)

closo-.

Tetrabutylammonium salt: [92227-35-5].

Synth. by heating under reflux $(Bu_4N)_2B_6H_6$ + nickelocene in MeCN. Cryst.

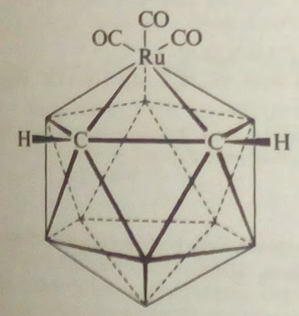
Vinitskii, D.M. *et al, Zh. Neorg. Khim.*, 1984, **29**, 1714 (*synth, ir, uv, pmr, B-11 nmr, ms*)

IC-004733

$C_5H_{11}B_9O_3Ru$

Tricarbonyl[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]ruthenium, 9Cl

[56465-06-6]



M 317.5

Yellow cryst. + ½ C_6H_6 (C_6H_6/cyclohexane). Mp >350°.

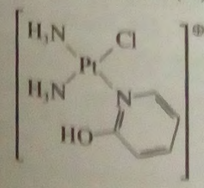
Seidle, A.R., *J. Organomet. Chem.*, 1975, **90**, 249 (*synth, ir, uv, nmr, pmr, ms*)

IC-004734

$C_5H_{11}ClN_3OPt^{\oplus}$

Diamminechloro[2(1*H*)-pyridinone]platinum(*II*)(1+), 1Cl

Diamminechloro(2-hydroxypyridine)platinum(II).
Diamminechloro(α-pyridone)platinum(II)



M 359.6 (ion)

Formed from pyridone, but struct. best considered as hydroxypyridine complex.

Chloride: [85336-86-3].

$C_5H_{11}Cl_2N_3OPt$ M 395.1

Amber cryst. Sol. aq. MeCN.

Nitrate: [86471-92-3].

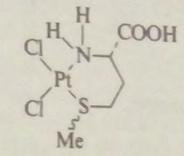
White needles.

Hollis, L.S. *et al, Inorg. Chem.*, 1983, **22**, 2708.

IC-004735

$C_5H_{11}Cl_2NO_2PtS$

Dichloro(methionine)platinum(*II*), 8Cl



(S)-methionine form

M 415.1

Chiral ligand. Carboxyl group not coordinated, possibly involved in intermolecular H-bonding.

(S)-methionine-form [31674-58-5]

(L-methionine)-form

Comprises mixt. of 2 stereoisomers due to chirality at S. Unresolved. Triclinic yellow cryst.

(±)-methionine-form [15654-80-5]

D,L-methionine-form

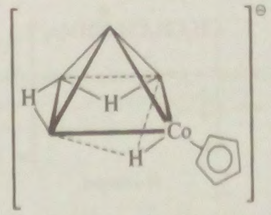
Synth. from (±)-methionine and K_2PtCl_4. Monoclinic yellow cryst. Insol. EtOH, Et_2O, Me_2CO, $CHCl_3$; mod. sol. hot H_2O (also reported insol. H_2O). Diamagnetic. Darkens at 230°.

Volshtein, L.M. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1963, **8**, 304 (*synth, props*)
McAuliffe, C.A., *J. Chem. Soc. A*, 1967, 641 (*ir*)
Erickson, L.E. *et al, J. Am. Chem. Soc.*, 1968, **90**, 6371 (*pmr*)
Freeman, H.C. *et al, J. Chem. Soc., Chem. Commun.*, 1970, 1523 (*cryst struct*)

IC-004736

$C_5H_{12}B_4Co^{\ominus}$

(η⁵-2,4-Cyclopentadien-1-yl)[heptahydrotetraborato(2−)]cobaltate(1−), 10Cl



M 174.3 (ion)

Used in synth. of larger clusters.

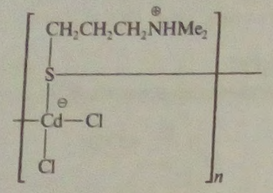
Na salt: [66102-08-7].

Sol. toluene, THF. Reacts with alkynes, $FeCO_3$, $CoCl_3/NaC_5H_5$.

Weiss, R. *et al, Inorg. Chem.*, 1978, **17**, 1522 (*synth, pmr, uses*)

$C_5H_{12}CdCl_2NS^{\ominus}$ IC-004737

Dichloro[3-(dimethylamino)-1-propanethiolato-*S*]cadmate(1−)



H-compd.

M 301.5 (ion)

H compd.: [111899-06-0]. *Dichloro[μ-(3-dimethylammonio-1-propanethiolato)]cadmate*
$C_5H_{13}CdCl_2NS$ M 302.5
Polymeric in solid state; isomorphous with Zn and Hg analogues. Cryst. (MeOH aq.).

Casals, I. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 2391 (*synth, ir, cryst struct*)

$C_5H_{12}ClO_3RhS_2$ IC-004738

Carbonylchlorobis(dimethyl sulfoxide)rhodium

Carbonylchlorobis[sulfinylbis[methane]-S]rhodium, 10CI

[74994-01-7]

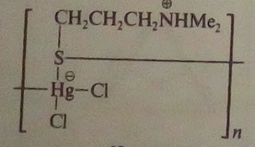
$(Me_2SO)_2RhCl(CO)$

M 322.6
Yellow solid. Sol. $CHCl_3$, Me_2CO. Mp 117-119° dec. Ir ν_{CO} 2020, ν_{SO} 1122, 1112 cm^{-1} (nujol).

Lawson, D.N. *et al, J. Chem. Soc.*, 1965, 1900 (*synth, ir*)
Dutta, D.K. *et al, Transition Met. Chem.*, 1980, **5**, 244 (*synth, ir, uv*)

$C_5H_{12}Cl_2HgNS^{\ominus}$ IC-004739

Dichloro[3-(dimethylamino)-1-propanethiolato-*S*]mercurate(1−)



H-compd.

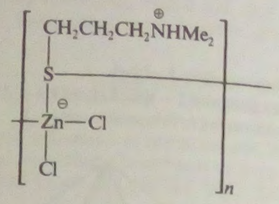
M 389.7 (ion)

H compd.: [111899-12-8]. *Dichloro[μ-(3-dimethylammonio)-1-propanethiolato]mercurate*
$C_5H_{13}Cl_2HgNS$ M 390.7
Cryst. (MeOH aq.). Polymeric in solid state.
Isomorphous with Zn and Cd analogues.

Casals, I. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 2391 (*synth, ir*)
Casals, I. *et al, Polyhedron*, 1988, **7**, 2509 (*cryst struct, ir, raman*)

$C_5H_{12}Cl_2NSZn^{\ominus}$ IC-004740

Dichloro[3-(dimethylamino)-1-propanethiolato-*S*]zincate(1−)



H-compd.

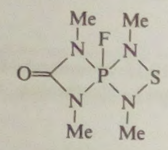
M 254.5 (ion)

H compd.: [111899-07-1]. *Dichloro[3-(dimethylammonio)-1-propanethiolato]zincate*
$C_5H_{13}Cl_2NSZn$ M 255.5
Polymeric in solid state: isomorphous with Cd and Hg analogues. Cryst. (aq. MeOH).

Casals, I. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 2391 (*synth, ir*)

$C_5H_{12}FN_4OPS$ IC-004741

4-Fluoro-1,3,5,7-tetramethyl-2-thia-1,3,5,7-tetraaza-4-phospha(4-*P*^{V})spiro[3.3]heptan-6-one



M 226.2

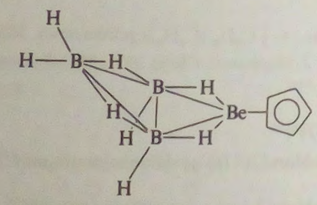
2,2-Dioxide: [21465-22-5].
Colourless cryst. (C_6H_6). Mp 116-118°. Begins to dec. at ca. 106°.

Becke-Goehring, M. *et al, Z. Anorg. Allg. Chem.*, 1969, **365**, 185 (*synth, pmr, F-19 nmr, P-31 nmr*)

$C_5H_{13}B_3Be$ IC-004742

(η⁵-2,4-Cyclopentadien-1-yl)[octahydrotriborato(1−)-*H*^{1},*H*^{3}]beryllium, 10CI

[66374-41-2]



M 114.6
Air- and moisture sensitive liq. (by trap-to-trap fractionation) at 0°. Sol. toluene. Fp 0°.

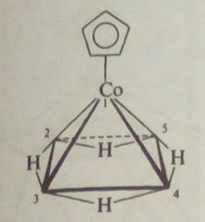
Gaines, D.F. *et al, Inorg. Chem.*, 1978, **17**, 1516 (*synth, ir, B-11 nmr, ms, pmr*)
Gaines, D.F. *et al, J. Magn. Reson.*, 1981, **44**, 84 (*Be-9 nmr*)

$C_5H_{13}B_4Co$ IC-004743

1-[(π-Cyclopentadienyl)cobalt]pentaborane(9)

1-[(π-Cyclopentadien-1-yl)[(1,2,3,4-η)-(η⁵-2,4-Cyclopentadien-1-yl)octahydrotetraborato(2−)]cobalt, 10CI

[43062-00-6]



M 175.3
nido-. Pale-yellow cryst. (by subl.). Sol. $CHCl_3$, CH_2Cl_2.

Miller, V.R. *et al, J. Am. Chem. Soc.*, 1973, **95**, 5078 (*synth*)
Miller, V.R. *et al, J. Am. Chem. Soc.*, 1977, **99**, 5646 (*synth, ir, nmr, ms*)
Brint, P. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1236 (*theory*)
Venable, T.L. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2275 (*synth, cryst struct, pmr, B-11 nmr, cmr*)

$C_5H_{13}B_4Co$ IC-004744

2-[(π-Cyclopentadienyl)cobalt]pentaborane(9)

(η⁵-2,4-Cyclopentadien-1-yl)[(1,2,3-η)-octahydrotetraborato(2−)-H^2,H^4]cobalt, 10CI

[43061-99-0]

M 175.3
nido-. Air-stable red cryst. (by subl.). Sol. $CHCl_3$.

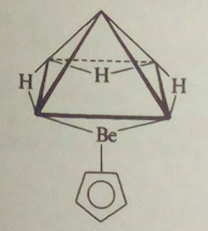
Miller, V.R. *et al, J. Am. Chem. Soc.*, 1973, **95**, 5078 (*synth*)
Sneddon, L.G. *et al, J. Chem. Soc., Chem. Commun.*, 1976, 118 (*struct*)
Miller, V.R. *et al, J. Am. Chem. Soc.*, 1977, **99**, 5646 (*synth, ir, nmr*)
Weiss, R. *et al, Inorg. Chem.*, 1978, **17**, 1522 (*props*)
Brint, P. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1236 (*theory*)
Venable, T.L. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2275 (*synth, pmr, B-11 nmr, cmr*)

$C_5H_{13}B_5Be$ IC-004745

(η⁵-2,4-Cyclopentadien-1-yl)[(2,3-η)-octahydropentaborato(1−)]beryllium, 10CI

μ-(η⁵-Cyclopentadienylberyllium)pentaborane(8)

[71163-79-6]



M 136.2
nido-. Air and moisture sensitive volatile colourless solid (purif. by trap-to-trap fractionation). V. sol. hydrocarbons, ethers, CH_2Cl_2. Mp 38°. V.p. << 1 mm at ambient temps.
▷ Expected to be toxic and pyrophoric.

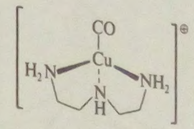
Gaines, D.F. *et al, J. Am. Chem. Soc.*, 1979, **101**, 3979 (*cryst struct, ms, B-11 nmr, pmr, synth*)
Gaines, D.F. *et al, Inorg. Chem.*, 1981, **20**, 2185 (*cryst struct, synth, B-11 nmr, pmr, deriv, props, ms*)

$C_5H_{13}CuN_3O^{\oplus}$ IC-004746

Carbonyl(diethylenetriamine)copper(1+)

[N-(2-Aminoethyl)-1,2-ethanediamine-N,N′,N″]carbonylcopper(1+)

[65832-81-7]



M 194.7 (ion)

Tetraphenylborate:
$C_{29}H_{33}BCuN_3O$ M 513.9
Mod. air-stable cryst. (MeOH). Sl. sol. THF, Me_2CO.

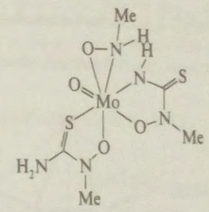
Pasquali, M. *et al, Inorg. Chem.*, 1978, **17**, 1684 (*synth, cryst struct*)

$C_5H_{13}MoN_5O_4S_2$ IC-004747

***N*-Methylhydroxylamido-*N,O*-(*N*-hydroxy-*N*-methylthioureato-*N,O*)-(*N*-hydroxy-*N*-methylthioureato-*O,S*)-oxomolybdenum(*VI*)**

(N-Hydroxymethanaminato-N,O)(N-hydroxy-N-methylthioureato-O,S)(N-hydroxy-N-methylthioureato(2−)-N′,O)oxomolybdenum(VI), 10CI

[74081-88-2]



M 367.2
7-Coordinate. Red cryst. Mp 127° dec.

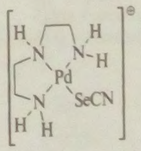
Wieghardt, K. *et al, Inorg. Chem.*, 1980, **19**, 2927 (*cryst struct*)

$C_5H_{13}N_4PdSe^{\oplus}$ IC-004748

(Diethylenetriamine)(selenocyanato)palladium(*II*)(1+)

[N-(2-Aminoethyl)-1,2-ethanediamine-N,N′,N″](selenocyanato-Se)palladium(1+)

[36656-87-8]



M 314.5 (ion)

Tetraphenylborate: [25930-61-4].
Light-yellow solid. Mp 144° dec. Stable with respect to linkage isomerisation.

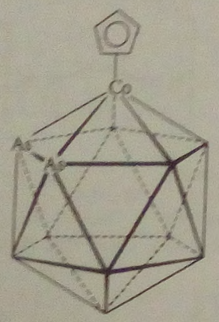
[36449-54-4]

Burmeister, J.L. *et al, J. Am. Chem. Soc.*, 1969, **91**, 44 (*synth, ir*)

$C_5H_{14}As_2B_9Co$ IC-004749

(η^5-2,4-Cyclopentadien-1-yl)(7,8,9,10,11-η)-nonahydro-7,8-diarsaundecaborato(2 –)]cobalt, 10CI

[65036-34-2]



M 380.2

closo-. Orange cryst. (CH_2Cl_2/heptane). Sol. CH_2Cl_2, Me_2CO. Mp 289-291°.

Little, J.L. *et al*, *Inorg. Chem.*, 1978, **17**, 584 (*synth, ir, pmr, B-11 nmr, us-vis*)

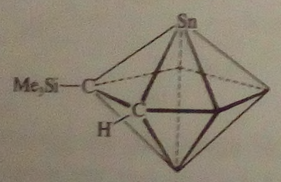
Geiger, W.E. *et al*, *Inorg. Chem.*, 1982, **21**, 2529 (*electrochem*)

$C_5H_{14}B_9SiSn$ IC-004750

2-(Trimethylsilyl)-2,3-dicarba-1-stannaheptaborane(6), 11CI

1-Stanna-2-(trimethylsilyl)-2,3-dicarba-closo-*heptaborane(6)*

[91686-40-7]



M 264.2

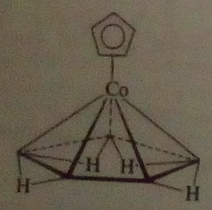
closo-. Off-white solid (by subl.). Sol. THF, Me_2CO. Mp 53-54°.

Hosmane, N.S. *et al*, *Organometallics*, 1984, **3**, 1665; 1986, **5**, 772 (*struct, synth, cmr, pmr, B-11 nmr, Si-29 nmr, Sn-119 nmr, ms*)

$C_5H_{14}B_5Co$ IC-004751

(η^5-2,4-Cyclopentadien-1-yl)[η^5-nonahydropentaborato(1 –)]cobalt, 10CI

[68457-41-0]



M 187.1

nido-. Mod. air-sensitive yellow cryst. (by low temp. vacuum fractionation at 0°). Sol. CH_2Cl_2.

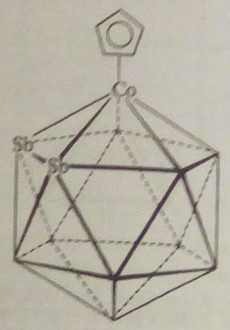
Wilczynski, R. *et al*, *Inorg. Chem.*, 1979, **18**, 864 (*synth, ir, pmr, B-11 nmr, ms*)

Brint, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 546 (*theory*)

$C_5H_{14}B_9CoSb_2$ IC-004752

(η^5-2,4-Cyclopentadien-1-yl)(7,8,9,10,11-η)-nonahydro-7,8-distibaundecaborato(2 –)]cobalt, 10CI

[69576-61-0]



M 473.8

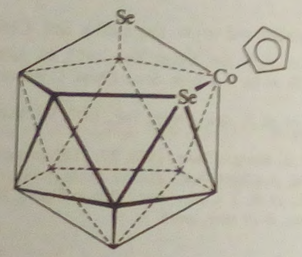
closo-. Yellow-orange solid. Sol. 1,2-dichloroethane, Me_2CO, CH_2Cl_2. Mp 296-298°.

Little, J.L., *Inorg. Chem.*, 1979, **18**, 1598 (*synth, pmr, B-11 nmr, ir*)

$C_5H_{14}B_9CoSe_2$ IC-004753

(η^5-2,4-Cyclopentadien-1-yl)[η^5-nonahydrodiselenaundecaborato(2 –)]cobalt, 10CI

[72207-08-0]



M 388.3

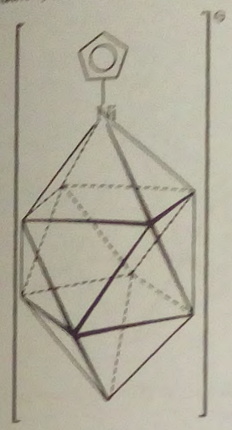
Dark green cryst. Sol. CH_2Cl_2, Me_2CO. Stable to at least 500°.

Friesen, G.D. *et al*, *Inorg. Chem.*, 1980, **19**, 458 (*synth, uv, pmr, cryst struct, B-11 nmr, ir*)

$C_5H_{16}B_9Ni^{\ominus}$ IC-004754

(η^5-2,4-Cyclopentadien-1-yl)[η^4-nonahydrononaborato(2 –)]nickelate(1 –), 9CI

(1-η^5-Cyclopentadienylnickel)nonahydrononaborate(1 –)



M 230.1 (ion)

Proposed struct. shown.

Me_4N salt: [57034-64-7].

Bright yellow solid (Me_2CO aq.). Sol. Me_2CO, MeCN.

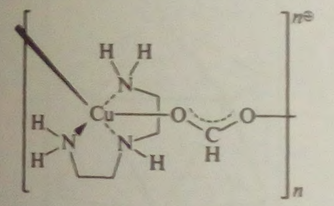
Sullivan, B.P. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 455 (*synth*)

Leyden, R.N. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 310 (*synth*)

Leyden, R.N. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3758 (*synth, nmr, ir*)

$C_5H_{16}CuN_3O_2^{\oplus}$ IC-004755

(Diethylenetriamine)-μ-formatocopper(*II*)(1 +)



M 211.7 (ion)

Square pyramidal coord. at copper. Chains of [Cu(dien)(HCO_2)]$^{\oplus}$ ions are formed by bridging formate groups.

Formate: [37072-98-3].

$C_6H_{15}CuN_3O_4$ M 256.7

Blue needles.

[29439-85-8, 31114-42-8, 32965-86-9]

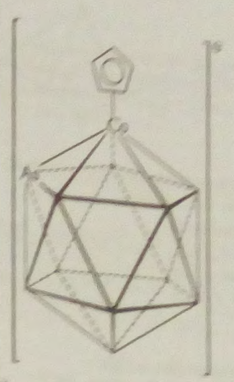
Davey, G. *et al*, *J. Chem. Soc. A*, 1971, 103 (*cryst struct*)

Bew, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1229 (*uv, ir, esr*)

$C_5H_{15}AsB_{10}Co^{\ominus}$ IC-004756

(η^5-2,4-Cyclopentadien-1-yl)(7,8,9,10,11-η)-1,2,3,4,5,6,8,9,10,11-decahydro-7-arsaundecaborato(2 –)]cobaltate(1 –), 10CI

[65015-72-7]



M 317.1 (ion)

closo-.

Me_4N salt: [65015-73-8].

Orange-brown cryst. (MeOH). Sol. Me_2CO, hot CH_2Cl_2, hot MeOH.

Little, J.L. *et al*, *Inorg. Chem.*, 1978, **17**, 584 (*synth, ir, pmr, B-11 nmr, us-vis*)

Geiger, W.E. *et al*, *Inorg. Chem.*, 1982, **21**, 2529 (*electrochem*)

$C_5H_{15}BO_2Si$ IC-004757

Dimethoxy(trimethylsilyl)borane, 11CI

[80476-78-4]

$Me_3SiB(OMe)_2$

M 146.0

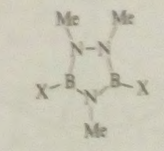
Biffar, W. *et al*, *Justus Liebigs Ann. Chem.*, 1981, 2067 (*synth, pmr, B-11 nmr*)

$C_5H_{15}B_2N_3$ IC-004758

1,2,3,4,5-Pentamethyl-1,2,4,3,5-triazadiborolidine, 10CI, 9CI

1,2,3,4,5-Pentamethyl-1,2,4,3,5-triazadiborolane

[31732-41-9]



X = Me

M 138.8

Liq., somewhat sensitive to moist air. $Bp_{2.5}$ 28°. ^{11}B nmr δ – 31.8 ppm.

Nölle, D. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1971, **10**, 126 (*synth, props, B-11 nmr*)

Nölle, D. *et al*, *Z. Naturforsch., B*, 1972, **27**, 1425.

Kroner, J. *et al*, *Chem. Ber.*, 1975, **108**, 3807 (*pe*)

Nöth, H. *et al*, *Chem. Ber.*, 1979, **112**, 2494 (*nmr, props*)

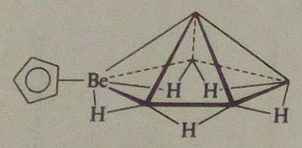
Füssstetter, H. *et al*, *Chem. Ber.*, 1980, **113**, 3881 (*struct*)

Goetze, R. *et al*, *Chem. Ber.*, 1981, **114**, 1884 (*B-11 nmr*)

$C_5H_{15}B_5Be$ IC-004759

(η^5-2,4-Cyclopentadien-1-yl)[decahydropentaborato(1 –)]beryllium

[65760-50-1]



M 138.2

nido-. Air and moisture sensitive volatile liq. (trapped at –20°). Sol. C_6H_6, toluene.

▷ Pyrophoric and toxic.

Gaines, D.F. *et al*, *Inorg. Chem.*, 1978, **17**, 1238 (*synth, ir, B-11 nmr, pmr, ms, props*)

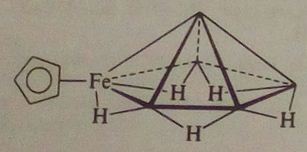
Bicerano, J. *et al*, *Inorg. Chem.*, 1979, **18**, 1565 (*theory*)

$C_5H_{15}B_5Fe$ IC-004760

(η^5-2,4-Cyclopentadien-1-yl)[η^3-decahydropentaborato(1 –)]iron, 10CI

2-(η^5-Cyclopentadienyl)-FeB_5H_{10}

[71661-61-5]



M 185.0

nido-. Air-sensitive violet cryst. (hexane). Therm. isom. to (η^5-2,4-Cyclopentadien-1-yl)[η^5-decahydropentaborato(1 –)]iron, IC-004761.

Weiss, R. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 8087.

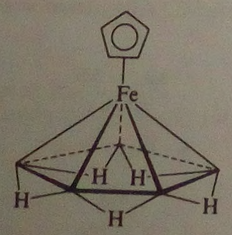
Weiss, R. *et al*, *Inorg. Chem.*, 1979, **18**, 3291 (*synth, pmr, nmr, ms*)

$C_5H_{15}B_5Fe$ IC-004761

(η^5-2,4-Cyclopentadien-1-yl)[η^5-decahydropentaborato(1 –)]iron, 10CI

1-(η^5-Cyclopentadienyl)-FeB_5H_{10}. Pentaboraferrocene

[65188-99-0]



M 185.0

nido-. Dark-violet air-sensitive solid.

Weiss, R. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 8087.

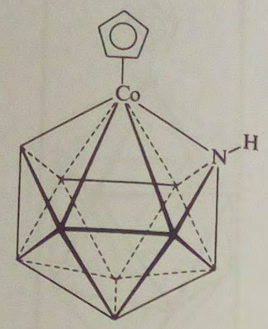
Weiss, R. *et al*, *Inorg. Chem.*, 1979, **18**, 3291 (*synth, pmr, nmr, ms*)

$C_5H_{15}B_9CoN$ IC-004762

(η^5-2,4-Cyclopentadien-1-yl)[(2,6,7,8,9,10-η)-decahydro-7-azadecaborato(2 –)]cobalt, 12CI

1-Cyclopentadienylcobalta-2-azaborane(11)

[117734-11-9]



M 245.4

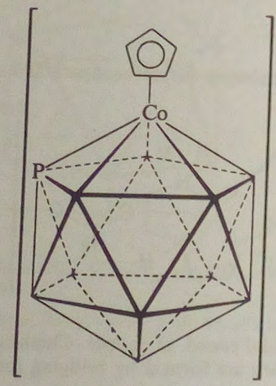
closo-. Blue-violet solid (CH_2Cl_2/pentane). Sol. THF, CH_2Cl_2, Me_2CO.

Koster, J.G. *et al*, *Inorg. Chem.*, 1988, **27**, 4528 (*synth, pmr, B-11 nmr, N-14 nmr, cryst struct*)

$C_5H_{15}B_{10}CoP^{\ominus}$ IC-004763

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-decahydro-7-phosphaundecaborato(2 –)]cobaltate(1 –), 9CI

1-(η^5-Cyclopentadienyl)-2-phospha-1-cobaltadodecaborate(1 –)



M 273.1 (ion)

Me_4N salt: [57091-20-0].

Orange-brown cryst. Sol. Me_2CO, THF, MeCN.

Little, J.L. *et al*, *Inorg. Chem.*, 1976, **15**, 114 (*synth, B-11 nmr, pmr, ir*)

$C_5H_{15}ClN_3Pt^{\oplus}$ IC-004764

[Bis(2-aminoethyl)methylamine]chloroplatinum(*II*)(1+)

(N-*2-Aminoethyl*-N-*methyl-1,2-ethanediamine*)*chloroplatinum(1+), 9CI. Chloro(4-methyl-1,4,7-triazaheptane)platinum*(II). *Chloro(1,5-diamino-3-methyl-3-azapentane)platinum*(II)

[59538-45-3]

As Bromo(diethylenetriamine)platinum(*II*), IC-004278 with

R = Me, X = Cl

M 347.7 (ion)

Suitable for study of mechanisms of Pt(*II*) substitutions.

Perchlorate: [59538-47-5].

Solid. Mp 261° dec.

▷ Potentially explosive.

Tetrachloroplatinate(2–) salt (2:1): [59538-46-4].

$C_{10}H_{30}Cl_6N_6Pt_3$ M 1032.3

Dark red cryst. Mp 273° dec.

Natile, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 626 (*synth, uv-vis*)

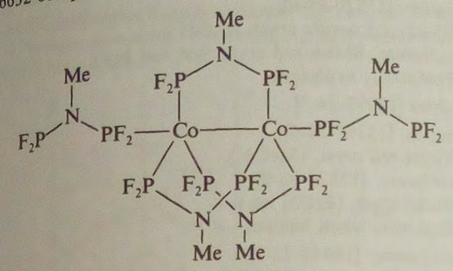
Annibale, G. *et al*, *Inorg. Chem.*, 1981, **20**, 2428 (*reactions*)

$C_5H_{15}Co_2F_{20}N_5P_{10}$ IC-004765

Pentakis(methylimidodiphosphorous tetrafluoride) dicobalt(0)

Tris[μ-(methylimidodiphosphorous tetrafluoride-P,P′)] bis(methylimidodiphosphorous tetrafluoride-P)dicobalt, 10CI. Pentakis[bis(difluorophosphino)methylamine]dicobalt(0)

[66632-81-3]



M 952.7

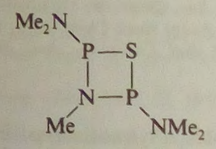
Black solid. Mp 140-142°.

King, R.B. *et al*, *Inorg. Chem.*, 1978, **17**, 2401 (*synth*)

$C_5H_{15}N_3P_2S$ IC-004766

2,4-Bis(dimethylamino)-3-methyl-1,3,2,4-thiazadiphosphetidine

N,N,N′,N′,3-Pentamethyl-1,3,2,4-thiazadiphosphetidin-2,4-diamine, 9CI



M 211.2

2,4-Disulfide: [55042-00-7].

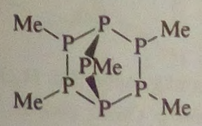
$C_5H_{15}N_3P_2S_3$ M 275.3

Solid. Mp 130-150°. Consists of a single stereoisomer.

Bulloch, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2329 (*synth, pmr, P-31 nmr*)

$C_5H_{15}P_7$ IC-004767

Pentamethylheptaphosphabicyclo[2.2.1]heptane, 11CI



M 291.9

Obt. as mixt. of steroeisomers. Synth. from PCl_3 + $(PMe)_5$ + Mg.

1,4-Dioxide (?): [102902-63-6].

Obt. by electrolysis of $MePCl_2/POCl_3/LiAlCl_4$ mixt.

[79180-89-5]

Baudler, M. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **473**, 20 (*synth, ir, ms, P-31 nmr*)

May, R. *et al*, *J. Electrochem. Soc.*, 1986, **133**, 855 (*synth, ms, P-31 nmr*)

$C_5H_{16}BNO$ IC-004768

[Dimethyl(2-methoxyethyl)amine]trihydroboron

Borane N,N-dimethyl(2-methoxyethyl)amine. Trihydro(2-methoxy-N,N-dimethylethanamine-N)boron, 10CI. Borane 2-methoxy-N,N-dimethylethylamine

[67036-07-1]

$MeOCH_2CH_2NMe_2—BH_3$

M 116.9

Used in electrolysis bath for Au and Pd coating.

Ger. Pat., 2 750 932, (1978); *CA*, **89**, 202734r (*use*)

U.S. Pat., 4 080 381, (1978); *CA*, **89**, 23753z.

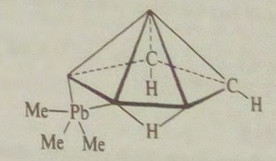
U.S. Pat., 4 142 902, (1979); *CA*, **91**, 25752p (*use*)

Ger. Pat., 3 000 526, (1980); *CA*, **94**, 19420z.

$C_5H_{16}B_4Pb$ IC-004769

2,3-μ-(Trimethylplumbyl)-4,5-dicarbahexaborane(8), 9CI

[38117-56-5]



M 326.6

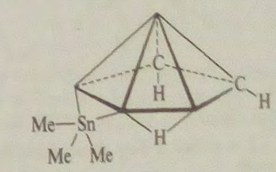
Proposed struct. shown. Colourless liq. of low volatility. Unstable at r.t.

Tabereaux, A. *et al*, *Inorg. Chem.*, 1973, **12**, 792 (*synth, nmr, pmr, ir*)

$C_5H_{16}B_4Sn$ IC-004770

2,3-μ-(Trimethylstannyl)-4,5-dicarbahexaborane(8), 9CI

[38117-56-5]



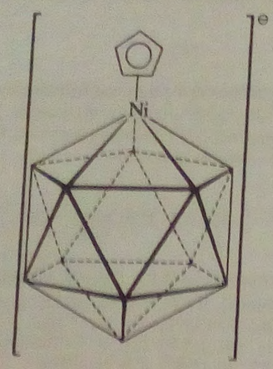
M 238.1

Colourless liq. Stable indefinitely at 120°, but dec. rapidly at 220°.

Tabereaux, A. *et al*, *Inorg. Chem.*, 1973, **12**, 792 (*synth, ir, pmr, nmr, ms*)

$C_5H_{16}B_{11}Ni^{\ominus}$ IC-004771

(η⁵-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydroundecaborato(2−)]nickelate(2−), 10CI



M 253.7 (ion)
closo-.

Me_4N salt: [55266-86-9].
Synth. from $Na_2B_{11}H_{13}$ + nickelocene in MeCN, followed by removal of solv., treatment with H_2O_2 and addition of Me_4NCl. Bright yellow needles (Me_2CO aq.) (63%).

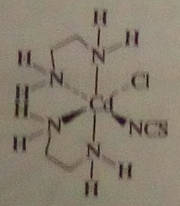
Hawthorne, M.F. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3758 (*synth, pmr, B-11 nmr, ir, electrochem*)

$C_5H_{16}CdClN_5S$ IC-004772

Chlorobis(ethylenediamine)isothiocyanatocadmium

*Chlorobis(1,2-ethanediamine-*N,N′*)(thiocyanato-*N*)cadmium, 9CI. Bis(1,2-ethylenediamine)cadmium chloride isothiocyanate*

[50989-71-4]



M 326.1
cis-Octahedral. Cryst.

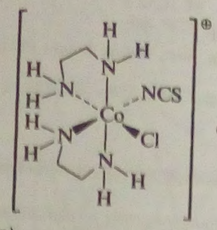
Shvelashvili, A.E. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **18**, 1133 (*synth*)
Shvelashvili, A.E. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1974, **15**, 315 (*cryst struct*)

$C_5H_{16}ClCoN_5S^{\oplus}$ IC-004773

Chlorobis(ethylenediamine)isothiocyanatocobalt(*III*)

*Chlorobis(1,2-ethanediamine-*N,N′*)(thiocyanato-*N*)cobalt*(III)(1+), *10CI*

[59538-16-8]



cis-form

M 272.6 (ion)

cis-form

Has been resolved.

Chloride: [13820-99-0].
Bluish-red needle cryst. (EtOH aq.).

Perchlorate: Bluish-red cryst. Sol. hot H_2O.
▷ Potentially explosive.

trans-form [16997-24-3]

Bromide: [15362-24-0].
Violet-red cryst. (MeOH).

Perchlorate: [13820-98-9].
Violet cryst. (EtOH aq.).
▷ Explosive when heated.

Thiocyanate: [16949-72-7].
Violet-blue cryst. (H_2O). Isomeric compd. $[Co(NCS)_2en_2]$ Cl (deep red) also exists.

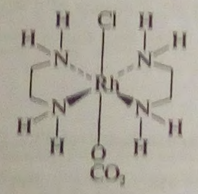
Werner, A., *Justus Liebigs Ann. Chem.*, 1912, **386**, 1, 139 (*synth, cis-form*)
Werner, A., *Justus Liebigs Ann. Chem.*, 1912, **386**, 57, 132, 169, 175 (*synth, trans-form*)
Gmelin Handbook Inorg. Chem., Syst. No. 58, 1930, **B**, 271; 1964, **B2**, 547 (*rev, bibl*)
Ingold, C.K. *et al*, *J. Chem. Soc.*, 1956, 1691 (*synth, reactions*)
Baldwin, M.E. *et al*, *J. Chem. Soc.*, 1960, 4275 (*cis-form, resoln, equation*)
Chottard, G., *Bull. Soc. Chim. Fr.*, 1973, 466 (*ir*)
House, D.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 219 (*cmr*)
Kanamori, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **53**, 2520 (*raman*)

$C_5H_{16}ClN_4O_3Rh$ IC-004774

Carbonatochlorobis(ethylenediamine)rhodium(*III*)

*[Carbonato(2−)-*O*]chlorobis(1,2-ethanediamine-*N,N′*)rhodium*(III), *10CI*

[75010-88-7]

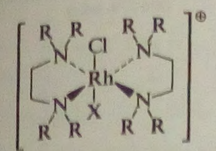


M 318.5
trans-Octahedral config. only. Sol. H_2O.

Van Eldik, R. *et al*, *Inorg. Chem.*, 1980, **19**, 3679 (*synth, uv, kinetics*)

$C_5H_{16}ClN_5RhS^{\oplus}$ IC-004775

Chlorobis(ethylenediamine)(thiocyanato-*N*)rhodium(*III*)(1+)



R = H , X = NCS

M 316.6 (ion)

trans-form

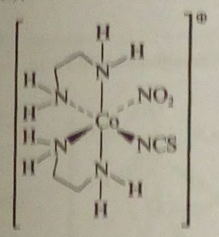
Thiocyanate: Bright yellow solid.

Johnson, S.A., *Inorg. Chem.*, 1962, **1**, 925 (*synth, uv*)

$C_5H_{16}CoN_6O_2S^{\oplus}$ IC-004776

Bis(ethylenediamine)(isothiocyanato)nitrocobalt(*III*)(1+)

*Bis(1,2-ethanediamine-*N,N′*)(nitrito-*N*)(thiocyanato-*N*)cobalt*(III)(1+), *11CI*



cis-form

M 283.2 (ion)
Nitrito to nitro linkage isomerisation of this complex has been studied.

cis-form

Chloride: Yellow-orange cryst. Sol. H_2O.

trans-form [86848-93-3]

No phys. props. reported. Sol. H_2O.

Chloride: No phys. props. reported.

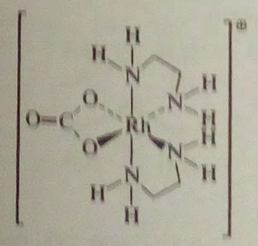
Adell, B., *Z. Anorg. Allg. Chem.*, 1952, **271**, 49 (*synth*)
Yamasaki, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 3060 (*cis-form*)
Miyoshi, K. *et al*, *Inorg. Chem.*, 1983, **22**, 1839 (*kinetics*)

$C_5H_{16}N_4O_3Rh^{\oplus}$ IC-004777

Carbonatobis(ethylenediamine)rhodium(*III*)(1+)

*[Carbonato(2−)-O,O′]bis(1,2-ethanediamine-*N,N′*)rhodium*(III)(1+), *10CI*

[72709-20-7]



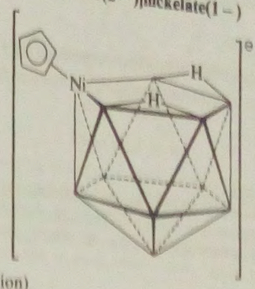
M 283.1 (ion)
Perchlorate: [72709-23-0].
Cream solid. Sol. H_2O.
▷ Potentially explosive.

Perchlorate, monohydrate: see *Aquacarbonatobis(ethylenediamine)rhodium*(III)(1+), IC-004792

Palmer, D.A. *et al*, *Inorg. Chem.*, 1980, **19**, 1009 (*synth, uv, kinetics*)

$C_5H_{17}B_{10}Ni^{\ominus}$

(η⁵-2,4-Cyclopentadien-1-yl)[η⁴-dodecahydrodecaborato(2−)]nickelate(1−) IC-004778



M 243.9 (ion)
nido-.

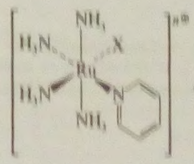
Me_4N salt: [67506-98-3].
Synth. from $NaB_{10}H_{13}$ + nickelocene + Na/Hg in 1,2-dimethoxyethane followed by addn. of Me_4NCl. Dark red cryst. (EtOH/Me_2CO). Sol. MeCN, Me_2CO.

H compd.: see *(η⁵-2,4-Cyclopentadien-1-yl)[η⁴-tridecahydrodecaborato(2−)]nickel*, IC-004790

Leyden, R.N. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3758 (*synth, pmr, B-11 nmr, ir, uv-vis, electrochem*)

$C_5H_{17}BrN_5Ru^{\oplus}$ IC-004779

Tetraammine(bromo)(pyridine)ruthenium(*II*)(1+), 9CI



n = 1 , X = Br

M 328.1 (ion)
Prepd. by the electrochemical reduction of the appropriate isomer of Tetraammine(bromo)(pyridine)ruthenium(*III*)(2+), IC-004780. Not isol. as salts. Sol. H_2O.

cis-form [63251-01-4]

trans-form [63323-60-4]

Marchant, J.A. *et al*, *Inorg. Chem.*, 1977, **16**, 2160 (*synth, uv, electrochem, equation*)

$C_5H_{17}BrN_5Ru^{2\oplus}$ IC-004780

Tetraammine(bromo)(pyridine)ruthenium(*III*)(2+)

As Tetraammine(bromo)(pyridine)ruthenium(*II*)(1+), IC-004779 with

n = 2, X = Br

M 328.1 (ion)
Sol. H_2O.

cis-form

Prepd. by treating *cis*-Tetraamminedi(aqua) ruthenium(*II*)(2+), IC-019965 with an equimolar amount of Py, followed by HBr, and oxidation with H_2O_2.

Dibromide: [63323-71-7].

trans-form

Prepd. by treating *trans*-Tetraammine(pyridine)[sulfato(2−)-*O*]ruthenium(*III*)(1+), IC-004787 in aq. HBr with Zn/Hg, followed by $BaCl_2$, and then H_2O_2.

Dibromide salt: [63251-14-9].

Marchant, J.A. *et al*, *Inorg. Chem.*, 1977, **16**, 2160 (*synth, uv, electrochem, aquation*)

$C_5H_{17}ClN_5Ru^{\oplus}$ IC-004781

Tetraammine(chloro)(pyridine)ruthenium(*II*)(1+), 9Cl

As Tetraammine(bromo)(pyridine)ruthenium(*II*)(1+), IC-004779 with

n = 1, X = Cl

M 283.7 (ion)

Pseudo-octahedral. Prepd. by the electrochemical reduction of the appropriate isomer of Tetraammine(chloro)(pyridine)ruthenium(*III*)(2+), IC-004782. Not isol. as salts. Sol. H_2O.

cis-form [63251-10-5]

trans-form [63323-67-1]

Marchant, J.A. *et al*, *Inorg. Chem.*, 1977, **16**, 2160 (*synth, uv, electrochem, aquation*)

$C_5H_{17}ClN_5Ru^{2\oplus}$ IC-004782

Tetraammine(chloro)(pyridine)ruthenium(*III*)(2+)

As Tetraammine(bromo)(pyridine)ruthenium(*II*)(1+), IC-004779 with

n = 2, X = Cl

M 283.7 (ion)

Sol. H_2O.

cis-form

Prepd. by treating *cis*-Tetraamminedi(aqua) ruthenium(*II*)(2+), IC-019965 with an equimolar amount of Py, followed by HCl, and oxidation with H_2O_2.

Dichloride: [63251-21-8].

trans-form

Prepd. by treating *trans*-Tetraammine(pyridine)[sulfato(2−)-*O*]ruthenium(*III*)(1+), IC-004787 in aq. HCl with Zn/Hg, followed by $BaCl_2$, and then H_2O_2.

Dichloride: [63251-20-7].

Pale yellow cryst.

Marchant, J.A. *et al*, *Inorg. Chem.*, 1977, **16**, 2160 (*synth, uv, electrochem, aquation*)

$C_5H_{17}IN_5Ru^{\oplus}$ IC-004783

Tetraammine(iodo)(pyridine)ruthenium(*II*)(1+)

As Tetraammine(bromo)(pyridine)ruthenium(*II*)(1+), IC-004779 with

n = 1, X = I

M 375.1 (ion)

Prepd. by the electrochemical reduction of the appropriate isomer of Tetraammine(iodo)(pyridine)ruthenium(*III*)(2+), IC-004784. Not isol. Sol. H_2O.

[63251-03-6, 63357-02-8]

Marchant, J.A. *et al*, *Inorg. Chem.*, 1977, **16**, 2160 (*synth, uv, electrochem, aquation*)

$C_5H_{17}IN_5Ru^{2\oplus}$ IC-004784

Tetraammine(iodo)(pyridine)ruthenium(*III*)(2+)

As Tetraammine(bromo)(pyridine)ruthenium(*II*)(1+), IC-004779 with

n = 2, X = I

M 375.1 (ion)

Sol. H_2O.

cis-form

Prepd. by treating *cis*-Tetraamminedi(aqua) ruthenium(*II*)(2+), IC-019965 with an equimolar amount of Py, followed by HI, and oxidation with H_2O_2.

Diiodide: [63323-73-9].

trans-form

Prepd. by treating Tetraammine(pyridine)[sulfato(2−)-*O*]ruthenium(*III*)(1+), IC-004787 with sat. aq. NaI.

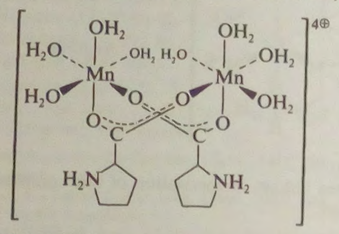
Diiodide: [63251-16-1].

Blue salt.

Marchant, J.A. *et al*, *Inorg. Chem.*, 1977, **16**, 2160 (*synth, uv, electrochem, aquation*)

$C_5H_{17}MnNO_6^{2\oplus}$ IC-004785

Tetraaqua(D,L-proline)manganese(*II*)(2+)



dimer

M 242.1 (ion)

Dimeric cation.

Sulfate (dimeric): [73796-73-3].

Synth. from aq. DL-proline and $MnSO_4$. Colourless plates (H_2O). Distorted octahedral Mn(*II*) complex built from $Mn(H_2O)_4^{2\oplus}$ and alternate layers of D- and L-proline zwitterionic molecules.

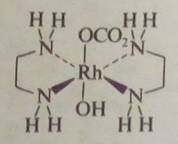
Ciunik, Z. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 693 (*synth, cryst struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 305 (*rev, bibl*)

$C_5H_{17}N_4O_4Rh$ IC-004786

Carbonatobis(ethylenediamine)hydroxyrhodium(*III*)

[*Carbonato*(2−)-O]*bis*(*1,2-ethanediamine*)*hydroxyrhodium*(III)



M 300.1

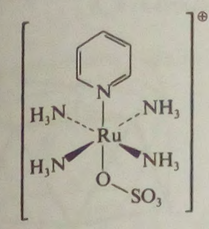
trans-form

Not isol., formed in soln. With CO_2, forms $Rh(en)_2(OCO_2)_2$.

Van Eldik, P., *Inorg. Chem.*, 1980, **19**, 3673 (*synth, uv*)

$C_5H_{17}N_5O_4RuS^{\oplus}$ IC-004787

Tetraammine(pyridine)[sulfato(2−)-*O*]ruthenium(*III*)(1+), 10Cl



M 344.3 (ion)

trans- Octahedral. Prepd. by oxidation of *trans*-$[Ru(NH_3)_4(Py)(SO_2)]^{2\oplus}$ in aq. HCl with H_2O_2.

Chloride: [63251-18-3].

Pale yellow salt.

Isied, S.S. *et al*, *Inorg. Chem.*, 1976, **15**, 3070 (*synth*)

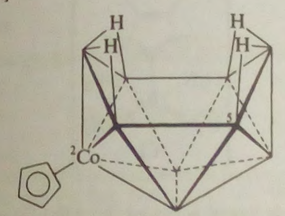
Curtis, J.C. *et al*, *Inorg. Chem.*, 1983, **22**, 224 (*synth*)

$C_5H_{18}B_9Co$ IC-004788

2-(η⁵-Cyclopentadienyl)-2-cobaltadecaborane(13)

2-(η⁵-2,4-Cyclopentadien-1-yl)[η⁵-tridecahydrononaborato(2−)*]cobalt*

[68457-40-9]



M 234.4

nido-. Synth. from $(C_5H_5)Co(CO)_2$ + B_5H_9. Air-stable orthorhombic yellow cryst. Sol. CH_2Cl_2. Mp 111-112°.

Wilczynski, R. *et al*, *Inorg. Chem.*, 1979, **18**, 864; 1980, **19**, 362 (*synth, ms, B-11 nmr, pmr*)

Zimmerman, G.J. *et al*, *Inorg. Chem.*, 1980, **19**, 3642 (*synth*)

Donohue, J. *et al*, *Cryst. Struct. Commun.*, 1981, **10**, 871 (*struct*)

$C_5H_{18}B_9Co$ IC-004789

5-(η⁵-Cyclopentadienyl)-5-cobaltadecaborane(13)

[43062-04-0]

M 234.4

nido-. Synth. from NaB_5H_8, $CoCl_2$ + NaC_5H_5. Red cryst. (hexane).

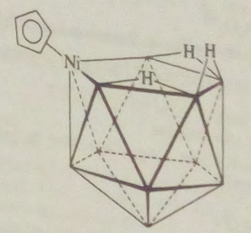
Grimes, R.N. *et al*, *Inorg. Chem.*, 1977, **16**, 3251 (*struct*)

Grimes, R.N. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 5646 (*B-11 nmr, synth, pmr*)

$C_5H_{18}B_{10}Ni$ IC-004790

(η⁵-2,4-Cyclopentadien-1-yl)[η⁴-tridecahydrodecaborato(2−)]nickel, 10Cl

[67564-09-4]



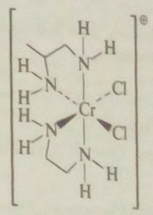
M 244.9

nido-. Bridging H's are fluxional. Synth. from nickelocene and decaborane in 1,2-dimethoxyethane. Red brown solid (C_6H_6). Sol. MeCN, Me_2CO.

Leyden, R.N. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3758 (*synth, pmr, B-11 nmr, ir, uv-vis, electrochem*)

$C_5H_{18}Cl_2CrN_4^{\oplus}$ IC-004791

Dichloro(1,2-ethanediamine-*N,N'*)(1,2-propanediamine-*N,N'*)chromium(*III*)(1+), 11Cl, 10Cl



cis-form

M 257.1 (ion)

cis-form

Chloride: [71884-67-8].

Obt. on heating *trans*-chloride at 140° for 1hr. Violet cryst. Sol. DMF.

trans-form

Converted to *cis*-form on heating.

Chloride: [71861-01-3].

Green cryst. + $\frac{1}{4}$ H_2O. Dehydrates at 70-160°.

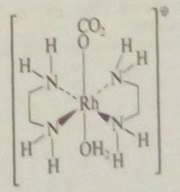
[67668-74-0]

Mitra, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 2569 (*synth, dta, isomers*)

$C_5H_{18}N_4O_4Rh^{\oplus}$ IC-004792

Aquacarbonatobis(ethylenediamine)rhodium(*III*)(1+)

Aqua[*carbonato*(2−)-O]*bis*(*1,2-ethanediamine*-N,N')*rhodium*(III)(*1+*), *10Cl*



M 301.1 (ion)

trans-Octahedral config. only.

Perchlorate: [75081-59-3].

Sol. H_2O.

▷ Potentially explosive.

Van Eldik, R. *et al*, *Inorg. Chem.*, 1980, **19**, 3673 (*synth, uv, kinetics*)

$C_5H_{19}CoN_4O_3^{2\oplus}$ IC-004793

Aquabis(ethylenediamine)formatocobalt(*III*)(2+)

$[Co(H_2NCH_2CH_2NH_2)_2(OH_2)(OOCH)]^{2\oplus}$

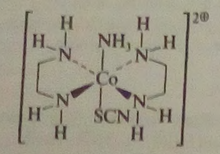
M 242.1 (ion)
Prepd. in soln. Not isol.

Kantrowiz, E.R. *et al*, *J. Phys. Chem.*, 1972, **76**, 2492 (*synth, photochem*)

$C_5H_{19}CoN_6S^{2\oplus}$ IC-004794

Amminebis(ethylenediamine)(thiocyanato-*S*)cobalt(*III*)(2+)

[25125-65-9]



M 254.2 (ion)
Octahedral, *cis*-form unknown. Base hydrolysis results in intramolecular rearrangement.

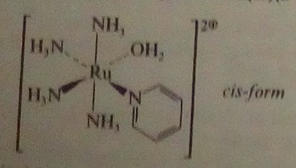
trans-form

Dichloride: [51976-69-3].
Purple lustrous cryst. Sol. H_2O.

Buckingham, D.A. *et al*, *Inorg. Chem.*, 1972, **11**, 2738 (*synth, ir, pmr*)

$C_5H_{19}N_5ORu^{2\oplus}$ IC-004795

Tetraammine(aqua)(pyridine)ruthenium(*II*)(2+), 9CI



cis-form

M 266.3 (ion)
Formed by the facile aquation of $[Ru(NH_3)_4(py)X]^{\oplus}$ (X = Cl, Br or I). H_2O ligand is readily displaced. Not isol. Sol. H_2O.

cis-form [26540-33-0]

trans-form [26518-89-8]

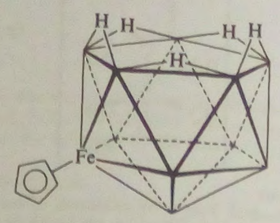
Ford, P.C. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 6209 (*photochem formn*)
Isied, S.S. *et al*, *Inorg. Chem.*, 1976, **15**, 3070 (*reactions*)
Marchant, J.A. *et al*, *Inorg. Chem.*, 1977, **16**, 2160 (*synth, uv, electrochem, reactions*)
Meade, T.J. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 4353 (*reaction, electrochem*)

$C_5H_{20}B_{10}Fe$ IC-004796

(η^5-2,4-Cyclopentadien-1-yl)[η^5-pentadecahydrodecaborato(2−)]iron, 10CI

2-(η^5-Cyclopentadienyl)-Fe$B_{10}H_{15}$

[71661-62-6]



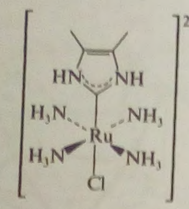
M 244.1
nido-. Yellow.

Weiss, R. *et al*, *Inorg. Chem.*, 1979, **18**, 3291 (*synth, pmr, nmr, ms*)

$C_5H_{20}ClN_6Ru^{2\oplus}$ IC-004797

Tetraamminechloro(1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene)ruthenium(2+), 9CI

Tetraammine(chloro)(4,5-dimethylimidazole)ruthenium(III)(2+)



M 300.7 (ion)
The imidazole ligand is bound through C(2) as an ylid; *trans*- octahedral at Ru. Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with 4,5-dimethylimidazole, followed by aerial oxidation in aq. HCl. Sol. H_2O.

Dichloride: [38959-98-7].
Purple cryst.

Sundberg, R.J. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 381 (*synth, uv*)

$C_5H_{20}ClN_{10}RuS_5^{2\oplus}$ IC-004798

Chloropentakis(thiourea-*S*)ruthenium(*III*)(2+), 9CI

[114110-39-3]

$[Ru[S{=}C(NH_2)_2]_5Cl]^{2\oplus}$ (C_{4v})

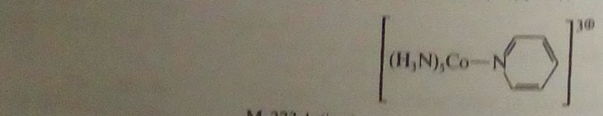
M 517.1 (ion)

Dichloride: Black solid. Mp 162°.

Taqui Khan, M.M., *J. Inorg. Nucl. Chem.*, 1973, **35**, 1395 (*synth*)
Rudnitskaya, O.V. *et al*, *Zh. Neorg. Khim.*, 1988, **33**, 140 (*synth*)

$C_5H_{20}CoN_6^{3\oplus}$ IC-004799

Pentaamminepyridinecobalt(*III*)(3+), 9CI



M 223.1 (ion)

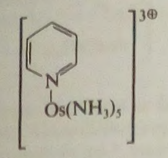
Triiodide: [35918-80-0].
Yellow cryst. Sol. H_2O.

Pritz, C.R. *et al*, *Inorg. Chem.*, 1973, **12**, 7 (*synth, ir, props*)

$C_5H_{20}N_6Os^{3\oplus}$ IC-004800

Pentaammine(pyridine)osmium(*III*)(3+)

[83781-38-8]



M 354.4 (ion)
Synth. e.g. from $[Os(NH_3)_5(OSO_2CF_3)](CF_3SO_3)_2$ and Py.

Trichloride: [70252-36-7].

Sen, J. *et al*, *Acta Chem. Scand., Ser. A*, 1979, **33**, 125 (*synth, ir, uv*)
Lay, P.A. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 7658 (*synth*)
Farquharson, S. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5123 (*raman, electrochem*)
Farquharson, S. *et al*, *Spectrochim. Acta*, Part A, 1984, **90**, 907.
Weaver, M.J. *et al*, *J. Chem. Phys.*, 1985, **82**, 4867 (*raman*)
Lay, P.A. *et al*, *Inorg. Chem.*, 1988, **27**, 2848 (*synth, uv*)
Harman, W.D. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5403 (*kinetics, electrochem*)

$C_5H_{20}N_6Ru^{2\oplus}$ IC-004801

Pentaammine(pyridine)ruthenium(*II*)(2+), 9CI

[21360-09-8]

$[Ru(NH_3)_5Py]^{2\oplus}$

M 265.3 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with Py. Sol. H_2O.

Diperchlorate: Yellow cryst.

Di-hexafluorophosphate: [72905-29-4].
Yellow cryst.

Ford, P. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 1187 (*synth, electrochem, uv, theory*)
Zwickel, A.M. *et al*, *Inorg. Chem.*, 1971, **10**, 2395 (*uv, theory*)
Allen, R.J. *et al*, *Inorg. Chem.*, 1972, **11**, 679 (*formn kinetics*)
Lavallee, D.K. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2583; 1977, **99**, 718 (*synth, uv, pmr, cmr*)
Shepherd, R.E. *et al*, *Inorg. Chem.*, 1973, **12**, 1392 (*formn kinetics*)
Ford, P.C., *Adv. Chem. Ser.*, 1978, **168**, 73 (*rev, photochem*)
Curtis, J.C. *et al*, *Inorg. Chem.*, 1983, **22**, 224 (*synth, uv, electrochem*)

$C_5H_{20}N_6Ru^{3\oplus}$ IC-004802

Pentaammine(pyridine)ruthenium(*III*)(3+), 10CI

[33291-25-7]

$[Ru(NH_3)_5(Py)]^{3\oplus}$

M 265.3 (ion)
Usually only generated in soln. Prepd. by oxidation of Ru(*II*) analogue. Disproportionates in basic soln. (pH ⩾ 8). Sol. polar solvs., H_2O. Underoges outer-sphere redox reactions with mild reducing agents.

Ford, P. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 1187 (*synth, uv*)
Ford, P. *et al*, *Inorg. Chem.*, 1969, **8**, 1544 (*uv*)
Gaunder, R.G. *et al*, *Inorg. Chem.*, 1970, **9**, 2627 (*synth, electrochem*)
Rudd, D.P. *et al*, *Inorg. Chem.*, 1971, **10**, 1543 (*disproportionation*)
Lim, H.S. *et al*, *Inorg. Chem.*, 1972, **11**, 1460 (*electrochem*)
Alvarez, V.E. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 7686 (*electrochem*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*synth, electrochem*)
Miralles, A.J. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 1416 (*reactions*)

$C_5H_{20}N_{10}O_7U^{2\oplus}$ IC-004803

Dioxopentakis(urea)uranium(*VI*)(2+)

$[UO_2[O{=}C(NH_2)_2]_5]^{2\oplus}$

M 570.3 (ion)
7-Coord. cation.

Diiodide: [21180-85-8]. *Uranyl iodide pentakis(urea)*
Yellow cryst. (H_2O). Sol. H_2O. Also obt. as monohydrate (red-orange cryst.).

Dinitrate: [17871-18-0]. *Uranyl nitrate pentakis(urea)*
Fluorescent blue-green cryst. Sol. H_2O. 7-Coord. pentagonal bipyramid at U.

Dodecachlorododecaborate: [77974-54-0].
Luminescent green-yellow cryst. V. sol. EtOH, Me_2CO, MeCN.

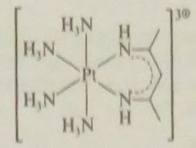
[7628-24-2]

Gentile, P.S. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 229 (*synth, ir*)
Tsapkina, I.V. *et al*, *Zh. Neorg. Khim.*, 1968, **13**, 1393; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 730 (*synth, ir*)
Ellert, G.V. *et al*, *Zh. Neorg. Khim.*, 1971, **16**, 3092; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1971, **16**, 1640 (*ir, luminescence*)
Seminara, A. *et al*, *Chim. Ind.* (*Milan*), 1976, **58**, 659; *CA*, **86**, 100159 (*synth*)
Zalkin, A. *et al*, *Inorg. Chem.*, 1979, **18**, 519 (*synth, cryst struct*)
Kuznetsov, N.T. *et al*, *Zh. Neorg. Khim.*, 1981, **26**, 1331; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1981, **26**, 715 (*synth*)
Mikhailov, Yu.N. *et al*, *Zh. Neorg. Khim.*, 1982, **27**, 2343; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 1321 (*cryst struct*)

$C_5H_{21}N_6Pt^{3\oplus}$ IC-004804

Tetraammine(2,4-pentanediiminato-*N,N'*)platinum(*IV*)(3+), 9CI

[56370-84-4]



M 360.3 (ion)
Synth. from $[Pt(NH_3)_6]^{2\oplus}$ + 2,4-pentanedione.

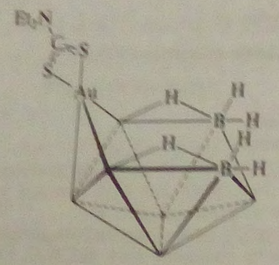
Triperchlorate: [61158-28-9].
Bright yellow cryst. (H_2O).
▷ Potentially explosive.

Evans, I.P., *J. Am. Chem. Soc.*, 1976, **98**, 8041 (*synth*)
Brawner, S.A. *et al*, *Inorg. Chem.*, 1978, **17**, 1304 (*pmr*)

$C_5H_{22}AuB_9NS_2$ IC-004805

[η^5-Dodecahydrooctaborato(2−)]-(diethylcarbamodithioato-*S,S'*)gold, 11Cl

[92389-04-3]



M 443.8

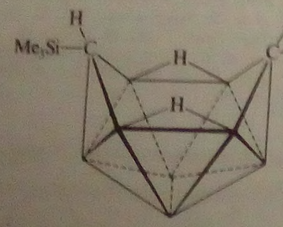
arachno-. Pale-yellow cryst. (CH_2Cl_2/pet. ether by chromatog.). Sol. CH_2Cl_2, $CHCl_3$, C_6H_6. See also [*μ*-[(3,4,5-*η*:6,7,8-*η*)-Decahydrooctaborato(2−)]]bis(diethylcarbamodithioato-*S,S'*)digold, IC-007192.

Beckett, M.A. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1427 (*synth, pmr, B-11 nmr*)

$C_5H_{22}B_9Si$ IC-004806

6-(Trimethylsilyl)-6,9-dicarbadecaborane(14)

[104761-15-1]



M 196.8

arachno-. Air-stable colourless cryst . (by subl. *in vacuo*). Sol. THF, Me_2CO, $CHCl_3$, CCl_4, CH_2Cl_2, C_6H_6.

Werner, J.R. *et al, Inorg. Chem.*, 1986, **25**, 4351 (*synth, pmr, B-11 nmr, cryst struct, ms, ir*)

$C_5H_{22}CoN_6O_2^{3\oplus}$ IC-004807

Pentaammine(ethyl cyanoacetate-*N*)cobalt(*III*)(3+), 10Cl

$[(H_3N)_5CoN{\equiv}CCH_2COOEt]^{3\oplus}$

M 257.2 (ion)

Nitrile ester probably coordinates through N.

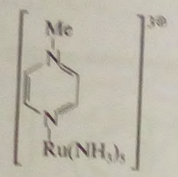
Triperchlorate: [69526-81-4].
Sol. DMSO, H_2O.
▷ Potentially explosive.

Creaser, I.I. *et al, J. Am. Chem. Soc.*, 1981, **103**, 3559 (*synth, ir, uv, pmr*)

$C_5H_{22}N_5Ru^{3\oplus}$ IC-004808

Pentaammine(*N*-methylpyrazinium-N^4)ruthenium(*II*)(3+)

[48135-76-8]



M 281.3 (ion)

Approx. octahedral at Ru. Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with *N*-methylpyrazinium 4-toluenesulfonate. Sol. H_2O.

Triperchlorate: Sol. H_2O.

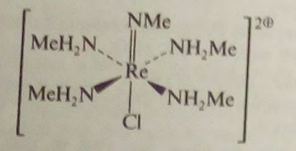
Tribromide: Violet-black hygroscopic crysts. $+2H_2O$ ($MeOH/H_2O$). Sol. H_2O.

Toma, H.E. *et al, J. Am. Chem. Soc.*, 1972, **94**, 4039 (*formn kinetics*)
Creutz, C. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1086 (*synth, uv, ir, electrochem*)
Malin, J.M. *et al, Inorg. Chem.*, 1975, **14**, 2924 (*pmr, cmr*)
Malouf, G. *et al, J. Am. Chem. Soc.*, 1977, **99**, 7213 (*photochem*)
Durante, V.A. *et al, Inorg. Chem.*, 1979, **18**, 588 (*flash photolysis*)
Moore, K.J. *et al, Inorg. Chem.*, 1983, **22**, 1108 (*electrochem*)
Fuerholz, U. *et al, Inorg. Chem.*, 1987, **26**, 3243 (*reaction*)
Winkler, J.R. *et al, J. Am. Chem. Soc.*, 1987, **109**, 2381 (*uv*)

$C_5H_{23}ClN_5Re^{2\oplus}$ IC-004809

Chlorotetrakis(methylamine)(methylimido)rhenium(*V*)(2+)

Chloro[methanaminato(2−)]tetrakis(methanamine)rhenium(V)(2+), *9Cl*



M 374.9 (ion)

Octahedral.

***trans*-form**

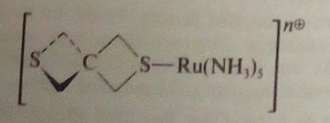
Interatomic distances: Re—Cl 240, Re=N 169, Re—N 216-219 pm.

Diperchlorate: [51014-18-7].
Deep blue cryst.
▷ Potentially explosive.

Shandles, R.S. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1869 (*synth, nmr*)
Shandles, R.S. *et al, Inorg. Chem.*, 1974, **13**, 1373 (*cryst struct*)

$C_5H_{23}N_5RuS_2^{2\oplus}$ IC-004810

Pentaammine[2,6-dithiaspiro[3.3]heptane-S^2]ruthenium(*II*)(2+)



$n = 2$

M 318.4 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with an excess of 2,6-dithiaspiro[3.3]heptane. Sol. H_2O, Me_2CO.

Bis-hexafluorophosphate: [76484-12-3].

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5H_{23}N_5RuS_2^{3\oplus}$ IC-004811

Pentaammine[2,6-dithiaspiro[3.3]heptane-S^2]ruthenium(*III*)(3+)

As Pentaammine[2,6-dithiaspiro[3.3]heptane-S^2]ruthenium(*II*)(2+), IC-004810 with

$n = 3$

M 318.4 (ion)

Prepd. by oxidation of the Ru(*II*) analogue with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5H_{23}ClCrN_5^{2\oplus}$ IC-004812

Chloropentakis(methylamine)chromium(*III*)(2+)

$[CrCl(NH_2Me)_5]^{2\oplus}$

M 242.7 (ion)

Severely distorted octahedral cation. Similar cations known with chloride replaced by e.g. Br, CF_3SO_3 and other amines.

Dichloride: [15351-84-5]. *Chromium*(III) *chloride pentakis-methylamine*
$C_5H_{23}Cl_3CrN_5$ M 313.6
Cryst.

Garner, C.S. *et al, Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Foxman, B.M., *Inorg. Chem.*, 1978, **17**, 1932 (*cryst struct*)
Lay, P.A., *J. Chem. Soc., Chem. Commun.*, 1986, 1422 (*aquation*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 787 (*rev*)

$C_5H_{25}ClN_5Rh^{2\oplus}$ IC-004813

Chloropentakis(methylamine)rhodium(*III*)(2+)

[64760-01-6]

$[RhCl(NH_2Me)_5]^{2\oplus}$

M 293.6 (ion)

Diperchlorate: [64760-02-7].
Yellow cryst. Sol. H_2O.
▷ Potentially explosive.

Swaddle, T.W. *et al, Can. J. Chem.*, 1977, **55**, 3166 (*synth, kinetics*)

$C_5H_{27}N_5RuS_2^{2\oplus}$ IC-004814

Pentaammine[1,3-bis(methylthio)propane-*S*]ruthenium(2+)

Pentaammine(2,6-*dithiaheptane*-S)*ruthenium*(II)(2+)

$[Ru(NH_3)_5S(Me)CH_2CH_2CH_2SMe]^{2\oplus}$

M 322.5 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with an excess of 2,6-dithiaheptane. Sol. H_2O, Me_2CO.

Bis-hexafluorophosphate: [76231-06-6].

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5H_{27}N_5RuS_2^{3\oplus}$ IC-004815

Pentaammine[1,3-bis(methylthio)propane-*S*]ruthenium(3+)

Pentaammine(2,6-*dithiaheptane*-S)*ruthenium*(III)(3+)

$[Ru(NH_3)_5S(Me)CH_2CH_2CH_2SMe]^{3\oplus}$

M 322.5 (ion)

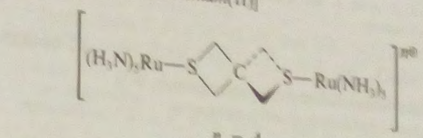
Prepd. by oxidation of the Ru(*II*) analogue with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5H_{38}N_{10}Ru_2S_2^{4\oplus}$ IC-004816

Decaammine[*μ*-[2,6-dithiaspiro[3.3]heptane-S^2:S^6]]diruthenium(4+)

μ-[2,6-*Dithiaspiro*[3.3]*heptane*]-*bis*[*pentaammineruthenium*(II)]



$n = 4$

M 504.6 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with 2,6-dithiospiro[3.3]heptane stoichiometrically. Sol. H_2O, Me_2CO.

Tetrakis-hexafluorophosphate: [76231-10-2].
No phys. props. reported.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5H_{38}N_{10}Ru_2S_2^{5\oplus}$ IC-004817

Decaammine[*μ*-[2,6-dithiaspiro[3.3]heptane-S^2:S^6]]diruthenium(5+)

μ-[2,6-*Dithiaspiro*[3.3]*heptane*]-*bis*[*pentammineruthenium*(II,III)]

[76723-23-4]

As Decaammine[*μ*-[2,6-dithiaspiro[3.3]heptane-S^2:S^6]]diruthenium(4+), IC-004816 with

$n = 5$

M 504.6 (ion)

Prepd. by oxidising Decaammine[*μ*-[2,6-dithiaspiro[3.3]heptane-S^2:S^6]]diruthenium(4+), IC-004816 with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5H_{42}N_{10}Ru_2S_2^{4\oplus}$ IC-004818

Decaammine[*μ*-[1,3-bis(methylthio)propane-*S*:*S'*]]diruthenium(4+)

μ-(2,6-*Dithiaheptane*)-*bis*[*pentaammineruthenium*(II)]

Decaammine[*μ*-(2,6-*dithiaheptane*-S:S')]*diruthenium*(4+)

$[(H_3N)_5Ru{-}S(Me)CH_2CH_2CH_2S(Me){-}Ru(NH_3)_5]^{4\oplus}$

M 508.7 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with 2,6-dithiaheptane stoichiometric. Sol. H_2O, Me_2CO.

Tetrakis-hexafluorophosphate: [76566-44-4].
No phys. props. reported.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5H_{42}N_{10}Ru_2S_2^{5\oplus}$ IC-004819

Decaammine[μ-1,3-bis(methylthio)propane-*S,S'*]diruthenium(5+)

μ-(2,6-Dithiaheptane)-bis[pentaammineruthenium(II,III)].

Decaammine[μ-(2,6-dithiaheptane-S:S')]diruthenium(5+)

$[(H_3N)_5Ru{-}S(Me)CH_2CH_2CH_2S(Me){-}Ru(NH_3)_5]^{5\oplus}$

M 508.7 (ion)

Prepd. by oxidizing Decaammine[μ-[1,3-bis(methylthio) propane-*S:S'*]]diruthenium(4+), IC-004818 with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 693 (*synth, uv, electrochem*)

$C_5HgIMnO_5$ IC-004820

Pentacarbonyl(iodomercury)manganese, 9CI

Pentacarbonyl(iodomercurio)manganese

[17524-67-3]

$IHgMn(CO)_5$

M 522.4

Synth. from $Hg[Mn(CO)_5]_2$ and HgI_2 in Me_2CO. Lemon-yellow needles (MeOH). Mp 135-136° dec. Ir ν_{CO} 2103m, 2043w, 2018vs cm^{-1} ($CHCl_3$).

Hieber, W. *et al*, *Chem. Ber.*, 1960, **93**, 455 (*synth, ir*)
Brier, P.N. *et al*, *J. Chem. Soc. A*, 1967, 1889 (*ir*)
Bower, L.M. *et al*, *J. Chem. Soc. A*, 1968, 706 (*ir*)
Hsieh, A.T.T., *Int. J. Mass Spectrom. Ion Phys.*, 1971, **7**, 319 (*ms*)

C_5IMnO_5 IC-004821

Pentacarbonyliodomanganese, 10CI

Iodopentacarbonylmanganese

[14879-42-6]

$MnI(CO)_5$ (C_{4v})

M 321.8

Synth. from $Na[Mn(CO)_5]$ and I_2 in THF. Red-orange cryst. (hexane). Subl.$_{0.05}$ 50°. Iodine is liberated on prolonged standing at r.t., dimerises slowly in soln.

Abel, E.W. *et al*, *J. Chem. Soc.*, 1959, 1501 (*synth, props*)
Kaesz, H.D. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 2844 (*ir*)
Connor, J.A. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 1754 (*props*)
Inorg. Synth., 1979, **19**, 160, 162 (*synth*)

$C_5IMoO_5^{\ominus}$ IC-004822

Pentacarbonyliodomolybdate(1−), 9CI

$(OC)_5MoI^{\ominus}$

M 362.8 (ion)

Et_4N salt: [14781-00-1].
Yellow cryst.

Bis(triphenylphosphine)iminium salt: [39004-14-3].
Yellow cryst.

Abel, E.W. *et al*, *J. Chem. Soc.*, 1963, 2068 (*synth*)
Ruff, J.K. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1972, **1**, 215 (*synth*)
Bond, A.M. *et al*, *Inorg. Chem.*, 1974, **13**, 602 (*props*)

$C_5IN_5Rh^{3\ominus}$ IC-004823

Pentakis(cyano-*C*)iodorhodate(*III*)(3−), 9CI

Pentacyanoiodorhodate(III)

$[Rh(CN)_5I]^{3\ominus}$ (C_{4v})

M 359.8 (ion)

Tri-K salt: [42892-96-6].
Sol. H_2O.

Hexaamminecobalt(3+) salt: [42892-98-8].
$C_5H_{18}CoIN_{11}Rh$ M 521.0
Yellow cryst. Sol H_2O.

Geoffroy, G.L. *et al*, *Inorg. Chem.*, 1974, **13**, 430 (*synth, ir, uv*)

C_5IO_5Re IC-004824

Pentacarbonyliodorhenium, 9CI

Iodopentacarbonylrhenium

[13821-00-6]

$IRe(CO)_5$ (O_h)

M 453.1

Synth. by uv irradiation of $Re_2(CO)_{10}$. Air-stable white cryst. by subl. Subl.$_{0.1}$ 85°. Ir ν_{CO} 2150w, 2045s, 2015w, 1990s cm^{-1} (CCl_4).

Junk, G.A. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 5758 (*ms*)
Colton, R. *et al*, *Aust. J. Chem.*, 1972, **25**, 9 (*synth, ir*)
Higginson, B.R. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1975, 1912 (*pe*)
Wrighton, M.S. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1111 (*uv*)
Vancea, L. *et al*, *J. Organomet. Chem.*, 1977, **134**, 219 (*synth, cmr*)
Kariuki, D.N. *et al*, *Inorg. Chem.*, 1978, **17**, 1018 (*ir, raman*)
Inorg. Synth., 1985, **23**, 44 (*synth, ir*)

C_5IO_5Tc IC-004825

Pentacarbonyliodotechnetium, 10CI

[15841-96-0]

$(OC)_5TcI$ (C_{4v})

M 365.8

No phys. props. recorded.

[41375-73-9]

Hileman, J.C. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2953 (*synth*)
DeJong, I.G. *et al*, *Inorg. Chem.*, 1973, **12**, 2519 (*synth*)
Behrens, R.G., *J. Less-Common Met.*, 1978, **61**, 321 (*thermodyn*)

C_5MnNO_8 IC-004826

Pentacarbonylnitratomanganese(*I*)

$Mn(ONO_2)(CO)_5$

M 256.9

Synth. from $Mn_2(CO)_{10}$ and N_2O_4 in pet. ether at 0°. Bright yellow powder, stable at r.t. for several weeks. Sol. HNO_3, $MeNO_2$, EtOH, $CHCl_3$, Me_2CO; spar. sol. C_6H_6, Et_2O, H_2O, CCl_4. Evolves CO on heating. Low spin Mn(*I*). Weak electrolyte. Undergoes substitution reactions with Py and bipy.

Addison, C.C. *et al*, *J. Chem. Soc.*, 1961, 4839 (*synth, ir, uv, magnetism, thermal stab, props*)

$C_5MnN_5^{3\ominus}$ IC-004827

Pentakis(cyano-*C*)manganate(*II*)(3−)

$[Mn(CN)_5]^{3\ominus}$

M 185.0 (ion)

Tri-K salt:
$C_5K_3MnN_5$ M 302.3
Synth. by reduction of $K_3Mn(CN)_6$ with H_2 at 420°. Brown solid. Insol. H_2O. $\mu_{eff} = 4.4\mu_B$. Struct. unknown, may have a Prussian blue-type struct.

Yoo, J.S. *et al*, *Inorg. Chem.*, 1965, **4**, 365 (*synth, ir, magnetism*)

Griffith, W.P., *Coord. Chem. Rev.*, 1975, **17**, 177 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, D3, 216 (*rev, bibl*)

$C_5MnN_6O^{3\ominus}$ IC-004828

Pentakis(cyano-*C*)nitrosylmanganate(*II*)(3−), 10CI

Pentacyanonitrosylmanganate(II)

[24868-90-4]

$[Mn(NO)(CN)_5]^{3\ominus}$ (C_{4v})

M 215.0 (ion)

Diamagnetic anion formulated as an Mn(*II*) complex with $CN^{\ominus}$ and NO ligands. Almost linear M—N—O. Anaerobic uv photolysis gives $[Mn(CN)_6]^{4\ominus}$ and NO but in presence of O_2, $[Mn(CN)_5(NO_2)]^{3\ominus}$ is formed. Oxidation with Br_2 or HNO_3 gives $[Mn(CN)_5NO]^{2\ominus}$. Reaction with $MeOSO_2F$ gives $[Mn(CNMe)_5NO][SO_3F]_2$. Slowly dec. in acid, neutral or alkaline soln. E° + 0.66V for $[Mn(CN)_5NO]^{2\ominus} + e^{\ominus} = [Mn(CN)_5NO]^{3\ominus}$.

Tri-K salt: [13821-02-8].
Synth. by storing $K_3[Mn(CN)_5NO].2H_2O$ and P_2O_5 under vacuum. Blue violet cryst. stable in air for up to 12 hrs. Insol. EtOH, Et_2O.

Tri-K salt dihydrate: [16009-97-5].
Synth. by adding NH_2OH to aq. Mn(*II*) salt and an excess of KCN. Purple cryst. (EtOH aq.) stable for 3 months in the absence of light. Diamagnetic, M—N 166, N—O 121 pm. Ir ν_{NO} 1706 cm^{-1}.

Tri-H compd.: [60255-50-7].
Synth. from $K_3[Mn(CN)_5NO].2H_2O$ in H_2O and conc. HCl at 0°. Carmine red cryst. (stable under dry N_2 for several days).

Tri-NH_4 salt, monohydrate: [67740-36-7].
Synth. by neutralising $H_3[Mn(CN)_5NO]$ with aq. NH_3. Violet cryst.

Tris-tetrabutylammonium salt: Synth. from $K_3[Mn(CN)_5NO]$ in H_2O with $[Bu_4N]Br$ in $CHCl_3$. Violet powder. Sol. $CHCl_3$.

Cotton, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1959, **10**, 28 (*synth, magnetism, ir, uv*)
Manoharan, P.T. *et al*, *Inorg. Chem.*, 1966, **5**, 823 (*synth, ir, uv*)
Jagner, S. *et al*, *Acta Chem. Scand.*, 1968, **22**, 3330 (*cryst struct*)
Miki, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 1024 (*ir*)
Poletti, A. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 2061 (*ir*)
Fenske, R.F. *et al*, *Inorg. Chem.*, 1972, **11**, 437 (*electronic struct*)
Mocák, J. *et al*, *J. Electroanal. Chem. Interfacial Electrochem.*, 1974, **57**, 369 (*electrochem*)
Mohai, B. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **441**, 263 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 252 (*rev, bibl*)

$C_5MnN_6O^{2\ominus}$ IC-004829

Pentakis(cyano-*C*)nitrosylmanganate(*III*)(2−), 10CI

Pentacyanonitrosylmanganate(III)

[25868-50-2]

$[Mn(NO)(CN)_5]^{2\ominus}$ (C_{4v})

M 215.0 (ion)

Paramagnetic anion with one unpaired electron formulated as an Mn(*III*) complex with $CN^{\ominus}$ and NO ligands. Synth. by oxidation of $[Mn(NO)(CN)_5]^{3\ominus}$. E° $[Mn(NO)(CN)_5]^{2\ominus} + e^{\ominus} = [Mn(NO)(CN)_5]^{3\ominus}$ + 0.597V.

Di-K salt: [13859-40-0].
Synth. from $K_3Mn(NO)(CN)_5$ in H_2O and either conc. HNO_3 or Cl_2. Canary yellow solid (Me_2CO/Et_2O) dec. in moist air. V. sol. H_2O; sol. EtOH; spar. sol. anhyd. Me_2CO. Solns. become cloudy in a few mins. μ_{eff} = 1.73μ_B at r.t. Ir ν_{NO} 1885 cm^{-1}.

Di-Ag(I) salt: [14516-53-1].
Synth. by oxid. of $[Mn(NO)(CN)_5]^{3\ominus}$ with HNO_3 and addition of $AgNO_3$. Light-brown to flesh coloured solid. Sl. sol. H_2O but solns. quickly dec. to AgCN and other prods. Ir ν_{NO} 1880, ν_{CN} 2175 cm^{-1} (approx. values).

Bis-tetrabutylammonium salt: [64914-10-9].
Synth. from $K_2Mn(NO)(CN)_5$ and $[Bu_4N]Cl$ in dry Me_2CO. Yellow solid.

Bis-Ph_4P salt: [64914-11-0].
Synth. from $K_2Mn(NO)(CN)_5$ and $[Ph_4P]Cl$ in H_2O. Yellow solid. Insol. H_2O. Ir ν_{NO} 1840 cm^{-1}.

Cotton, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1959, **10**, 28 (*synth, ir, uv, magnetism*)
Manoharan, P.T. *et al*, *Inorg. Chem.*, 1966, **5**, 823 (*synth, ir, uv, esr*)
Miki, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 1024 (*ir*)
Folkesson, B., *Acta Chem. Scand., Ser. A*, 1974, **28**, 491 (*ir*)
Griffith, W.P., *Coord. Chem. Rev.*, 1975, **17**, 177 (*rev, bibl*)
Papp, S. *et al*, *Magy. Chem. Foly.*, 1977, **83**, 346; *CA*, **87**, 210398 (*synth, ir, props*)
Mohai, B. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **441**, 263 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 271 (*rev, bibl*)

$C_5MnO_5^{\ominus}$ IC-004830

Pentacarbonylmanganate(1−), 10CI

[14971-26-7]

$[Mn(CO)_5]^{\ominus}$

M 194.9 (ion)

Li salt: [15689-01-7].
C_5LiMnO_5 M 201.9
Moisture-sensitive.

Na salt: [13859-41-1].
C_5MnNaO_5 M 217.9
Moisture-sensitive white cryst. Turns deep-green between 122° and 125°. Ir ν_{CO} 1896s, 1863vs cm^{-1} (HMPA).

K salt:
C_5KMnO_5 M 234.0
Moisture-sensitive.

Me_4N salt: Bright-yellow microcryst. (THF). Ir ν_{CO} 1899s, 1867s cm^{-1} (THF).

Bis(triphenylphosphine)iminium salt: [52542-59-3].
Orange cryst.

Triamminetricarbonylmanganese(1+) salt: [67315-40-6].
Yellow cryst. (Et_2O/pentane). Mp 150° dec. Ir ν_{CO} 2025m, 1908vs, 1858br cm^{-1} (THF).

Inorg. Synth., 1974, **15**, 84 (*synth*)
Herberhold, M. *et al*, *J. Organomet. Chem.*, 1978, **152**, 329 (*struct, ir, cmr, pmr*)
Gladysz, J.A. *et al*, *Inorg. Chem.*, 1979, **18**, 553 (*synth*)
Duffy, D.N. *et al*, *J. Organomet. Chem.*, 1979, **164**, 227 (*props*)
Pearson, R.G. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 1541 (*props*)
Casey, C.P. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 2728 (*synth, ir*)
Uson, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 316 (*props*)
Braunstein, P. *et al*, *J. Organomet. Chem.*, 1981, **213**, 79 (*props*)
Moore, E.J. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 2257 (*ir*)
Organomet. Synth., 1988, **4**, 101 (*synth, ir*)

C_5MnO_5Tl IC-004831

Pentacarbonyl(thallium)manganese, 9CI

Pentacarbonylmanganesethallium

[52720-99-7]

$TlMn(CO)_5$

M 399.3

Disproportionates in soln. to $Tl[Mn(CO)_5]_3$. Synth. from TlOEt and $HMn(CO)_5$. Generated and used as THF soln. Ir ν_{CO} 2029m, 1921vs cm^{-1} (THF).

Burlitch, J.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 828 (*synth, ir*)

$C_5MnO_7S^{\oplus}$ IC-004832

Pentacarbonyl(sulfur dioxide-*S*)manganese(1+)

$[Mn(CO)_5(SO_2)]^{\oplus}$

M 259.0 (ion)

Hexafluoroarsenate: [55853-06-0].
Synth. from $MnBr(CO)_5$, $AgAsF_6$ and SO_2. Brownish-yellow solid. Dec. in high vacuum at r.t. to give $MnF(CO)_5.AsF_5$. Reacts with $MnBr(CO)_5$ to give $[(OC)_5MnBrMn(CO)_5]AsF_6$.

Mews, R., *Angew. Chem., Int. Ed. Engl.*, 1975, **14**, 640; 1977, **16**, 56 (*synth*)

$C_5NO_5ReS^{2\oplus}$ IC-004833

Pentacarbonyl(thionitrosyl)rhenium(2+), 11CI

$[Re(CO)_5(NS)]^{2\oplus}$

M 372.3 (ion)

Bis-hexafluoroantimonate: [84303-53-7].
Light-red solid. Sl. sol. SO_2. Dec. at 136°. Ir ν_{CO} 2220vs, 2200w, 2178sh, 2160vs, 2068m, 2038sh; Ir ν_{NS} 1370vs cm^{-1}(nujol/Kel-F).

Hartmann, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 202.
Hartmann, G. *et al*, *Z. Naturforsch., B*, 1985, **40**, 343 (*synth, ir*)

C_5NO_6V IC-004834

Pentacarbonylnitrosylvanadium, 11CI

[14883-03-5]

$V(CO)_5NO$

M 221.0

Synth. by reaction of $[Et_4N][V(CO)_6]$ and $[NO][BF_4]$ in CH_2Cl_2 at −50°. Highly reactive, CO readily replaced by other ligands. Thermally unstable deep red-violet cryst., may be stored for weeks at −25° under N_2. Sol. CH_2Cl_2, aromatic hydrocarbons. Dec. >10°. Ir ν_{CO} 2100w, 2050w, 1990s, ν_{NO} 1695 cm^{-1} (hexane).

Fjare, K.L. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 2303 (*synth, ir, ms, uv, bibl*)

$C_5N_5NbOS_5^{2\ominus}$ IC-004835

Oxopentakis(thiocyanato-*N*)niobate(*V*)(2−), 11CI

Pentaisothiocyanatooxoniobate(V)(2−).
Pentakis(isothiocyanato)oxoniobate(V)(2−), *8CI*

[21791-70-8]

$[NbO(NCS)_5]^{2\ominus}$ (C_{4v})

M 399.3 (ion)

Octahedral. Formed in a spectrophotometric estimation of Nb.

Bis-Et_4N salt: [58179-28-5].
Yellow solid. Mp 228-235°. Ir $\nu_{Nb=O}$ 935 cm^{-1}.
Bis-Ph_4P salt: [58288-60-1].
Yellow solid. Mp 261-265°. Ir $\nu_{Nb=O}$ 935 cm^{-1}.
Bis-Ph_4As salt: [30267-08-4].
Synth. by reaction of Nb(*V*) solns. with excess KNCS, extracting with Et_2O and adding $[Ph_4As]Cl$ to the extract. Dark yellow solid. Mp 258-261°. Nb—O 170 pm. Ir $\nu_{Nb=O}$ 935 cm^{-1}.

Djodjević, C. *et al*, *Anal. Chem.*, 1968, **40**, 1512 (*synth, Nb detn*)
Kamenar, B. *et al*, *J. Chem. Soc. A*, 1970, 2379 (*cryst struct*)
Tamhina, B. *et al*, *Croat. Chim. Acta*, 1975, **47**, 79 (*synth, ir*)

$C_5N_5Ni^{3\ominus}$ IC-004836

Pentakis(cyano-*C*)nickelate(*II*)(3−)

Pentacyanonickelate(II)(3−), *8CI*

[29130-88-9]

$[Ni(CN)_5]^{3\ominus}$

M 188.7 (ion)

Synth. from $[Ni(CN)_4]^{2\ominus}$ + $CN^{\ominus}$.

Tris(1,2-ethanediamine)chromium(3+) salt, anhydrous: [30207-43-3].
$C_{11}H_{24}CrN_{11}Ni$ M 421.0
Square pyramidal anion. Red solid.
Tris(1,2-ethanediamine)chromium(3+) salt, 1.5 hydrate: [20523-47-1].
$C_{11}H_{27}CrN_{11}NiO_{1.5}$ M 448.0
Square pyramidal and trigonal bipyramidal nickel anions. Red cryst.
Tris(1,3-propanediamine)chromium(3+) salt, dihydrate: [52154-76-4].
$C_{14}H_{34}CrN_{11}NiO_2$ M 499.1
Square pyramidal anion. Red cryst.

Raymond, K.N. *et al*, *Inorg. Chem.*, 1966, **5**, 949; 1968, **7**, 1362 (*synth, ir, uv, cryst struct*)
Jurnak, F.A. *et al*, *Inorg. Chem.*, 1974, **13**, 2387 (*synth, cryst struct*)

$C_5N_5ORe S_5^{2\ominus}$ IC-004837

Oxopentakis(thiocyanato-*N*)rhenate(*V*)(2−), 10CI

Penta(isothiocyanato)oxorhenate(V)(2−)

$[ReO(NCS)_5]^{2\ominus}$

M 492.6 (ion)

Synth. from $ReO_4^{\ominus}$ and $NCS^{\ominus}$ ion or from $[ReOBr_4.MeCN]^{\ominus}$ or $ReOCl_5^{2\ominus}$ by ligand substitution.

Bis-tetrabutylammonium salt: [74176-28-6].
Yellow cryst.
Bis-Ph_4As salt: [74176-29-7].
Yellow-green cryst. (Me_2CO/isobutanol). Appears to exist in 2 cryst. forms.

Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 1160 (*synth, ir, uv, props*)

$C_5N_5OS_5Tc^{2\ominus}$ IC-004838

Pentakis(thiocyanato-*N*)oxotechnetate(*V*)(2−)

Penta(isothiocyanato)oxotechnetate(V)(2−)

$[TcO(NCS)_5]^{2\ominus}$ (C_{4v})

M 405.3 (ion)

Prep. from $TcOCl_4^{\ominus}$ + $NCS^{\ominus}$. Thiocyanate dissociates in dil. soln. (MeCN); in presence of excess $NCS^{\ominus}$ gives $Tc(NCS)_6^{n\ominus}$ complexes.

Bis-Ph_4As salt: [74185-18-5].

Red microcryst.

Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 1160 (*synth, uv, ir, magnetism, props*)

$C_5N_5OS_5V^{3\ominus}$ IC-004839

Oxopentakis(thiocyanato-*N*)vanadate(*IV*)(3−), 11CI

Pentaisothiocyanato(oxo)vanadate(IV)(3−)

[27342-93-4]

$[VO(NCS)_5]^{3\ominus}$ (C_{4v})

M 357.3 (ion)

Tris-Me_4N salt: [22608-76-0].
Synth. by adding excess $[Me_4N]NCS$ to $VO^{2\ominus}$ in H_2O. Dark blue solid.
Tris(methyltrioctylammonium) salt: [60551-56-6].
Synth. analogously to the Me_4N salt. May be used to extract V into C_6H_6. Blue solid.

Robbins, D.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 813 (*cd, mcd*)
Sato, T. *et al*, *Anal. Chim. Acta*, 1976, **84**, 397 (*synth, use*)
Johnson, M.D. *et al*, *Inorg. Chem.*, 1983, **22**, 1068 (*synth, Me_4N salt*)

$C_5N_5OTc^{2\ominus}$ IC-004840

Pentakis(cyano-*C*)oxotechnetate(*V*)(2−)

Pentacyanooxotechnetate(V)(2−)

$[O{=}Tc(CN)_5]^{2\ominus}$ (C_{4v})

M 244.9 (ion)

Octahedral anion. Product of aerobic hydrolysis of $Tc^{III}/CN^{\ominus}$ solns.; synth. by reaction of TcO_2 aq. with hot aq. KCN. Hydrol. to $[TcO_2(CN)_4]^{3\ominus}$.

Di-K salt: [73396-80-2].
Pale greenish-yellow cryst. (KCN aq.).

Trop, H.S. *et al*, *Inorg. Chem.*, 1980, **19**, 1993 (*synth, uv, ir, props*)

$C_5N_5OV^{3\ominus}$ IC-004841

Pentakis(cyano-*C*)oxovanadate(*IV*)(3−), 11CI

Pentacyanooxovanadate(IV)(3−).
Oxopentacyanovanadate(IV)(3−)

[26062-62-4]

$[VO(CN)_5]^{3\ominus}$ (C_{4v})

M 197.0 (ion)

Octahedral.

▷ Cyanides are toxic.

Tri-K salt: [32241-24-0].
Synth. by adding $VO(OAc)_2$ to saturated aq. KCN. Green solid. Paramagnetic; μ_{eff} = 1.64μ_B, g = 1.941.
Tri-Cs salt: [18866-26-7].
Synth. by adding CsCl to a soln. of $VOSO_4$ in 6*M* NaCN. Blue solid.
Tris-Me_4N salt: [36921-00-3].
Synth. by adding $[Me_4N]I$ to a soln. of $VOSO_4$ in 6*M* NaCN. Catalyst in a slurry process for the conversion of black oil. Light green solid.

Selbin, J. *et al*, *J. Inorg. Nucl. Chem.*, 1962, **24**, 1111 (*synth, Cs salt*)
Wasson, J.R., *J. Inorg. Nucl. Chem.*, 1968, **30**, 171 (*ir, uv-vis, Cs salt*)
Bennett, B.G. *et al*, *J. Chem. Soc. A*, 1971, 1204 (*synth, ir, uv-vis, K salt*)
U.S. Pat., 3 657 111, (1972); *CA*, **77**, 22545y (*use*)
Jagner, S. *et al*, *Acta Chem. Scand.*, 1973, **27**, 3482 (*cryst struct, K salt*)
Collison, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 667 (*uv-vis, K salt*)

$C_5N_5O_2S_5U^{3\ominus}$ IC-004842

Dioxopentakis(thiocyanato-*N*)uranate(*VI*)(3−)

Pentakis(isothiocyanato)dioxouranate(VI)(3−)

$[UO_2(NCS)_5]^{3\ominus}$

M 560.4 (ion)

Tri-K salt: Orange cryst. + $2H_2O$. Sol. H_2O, Me_2CO, MeOH, EtOH. Mp 235° dec. Loses H_2O on storage over conc. H_2SO_4 or on heating to 140-145°.
Tri-Cs salt: Orange cryst. + $2H_2O$. Sol. H_2O, MeOH, EtOH, Me_2CO. Mp 280° dec. Loses H_2O on storage over conc. H_2SO_4.
Tri-NH_4 salt: Orange cryst. + $2H_2O$. Sol. H_2O, Me_2CO, EtOH, MeOH. Mp 190° dec. Loses H_2O on storage over conc. H_2SO_4 or on heating to 80-90°.
Tris-Et_4N salt: Yellow solid + $1H_2O$. Sol. H_2O, EtOH. Mp 235-250°. Loses H_2O at 80-90°.
Tri-pyridinium salt: Yellow needles. Sol. EtOH, H_2O.

Markov, V.P. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1960, **5**, 712; 1960, **5**, 724; 1964, **9**, 305 (*synth*)
Arutgunyan, E.G. *et al*, *J. Struct. Chem. USSR (Engl. Transl.)*, 1963, **4**, 96 (*synth*)
Andrä, K. *et al*, *Z. Chem.*, 1965, **5**, 145 (*synth*)

$C_5N_5Zr^{5\ominus}$ IC-004843

Pentakis(cyano-*C*)zirconate(5−), 11CI

$[Zr(CN)_5]^{5\ominus}$

M 221.3 (ion)

Penta-K salt: [62278-13-1].
$C_5K_4N_5Zr$ M 416.8
Synth. from KCN and $ZrBr_3$ in liq. NH_3. Air-and moisture-sensitive grey powder. Insol. NH_3, gen. insol. in solvs. with which there is no reaction. μ_{eff} = 2.69μ_B (298K).

▷ Cyanides are toxic.

Nicholls, D. *et al*, *Inorg. Chim. Acta*, 1977, **21**, L17 (*synth, ir, powder struct*)

$C_5N_6ORe^{3\ominus}$ IC-004844

Pentakis(cyano-*C*)nitrosylrhenate(3−)

Pentacyanonitrosylrhenate(3−)

[69290-64-8]

$[Re(CN)_5(NO)]^{3\ominus}$

M 346.3 (ion)

$[Re(CN)_7NO]^{3\ominus}$ has been reformulated as above. Several salts known.

Tri-K salt: [69290-63-7].
Red cryst. + $3H_2O$ (H_2O). Sol. H_2O. Ir ν_{NO} ~1650 cm^{-1}. Diamagnetic.

[45047-06-1, 58601-85-7]

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1411 (*synth, ir, props*)

$C_5N_6ORu^{2\ominus}$ IC-004845

Pentakis(cyano-*C*)nitrosylruthenate(2−), 9CI

Pentacyano(nitrosyl)ruthenate(2−)

[34849-73-5]

$[Ru(CN)_5(NO)]^{2\ominus}$

M 261.1 (ion)
Approx. octahedral. Prep. by treating $[Ru(CN)_4]^{4\ominus}$ with HNO_3 or with NO. Reacts with base to give $[Ru(NO_2)(CN)_5]^{4\ominus}$.
Di-Li salt: Prep. by treating $Ag_2[Ru(NO)(CN)_5]$ with LiCl. Red salt. Readily sol. H_2O.
Di-Na salt: Prepd. by dehydrating the corresp. dihydrate over P_2O_5. Red-brown solid. Insol. H_2O.
Di-K salt: Prepd. by dehydrating corresp. dihydrate over P_2O_5. Red-brown solid. Insol. H_2O. Ir $\nu_{C\equiv N}$ 2200, 2145, 2100; ν_{NO} 1915 cm^{-1} (nujol).
Di-K salt, dihydrate: Ir $\nu_{C\equiv N}$ 2205, 2157, 2110, ν_{NO} 1927 cm^{-1} (KBr).
Di-Ag(I) salt:
$C_5Ag_2N_4ORu$ M 476.9
Prepd. by heating $K_4[Ru(CN)_5]$ with conc. HNO_3, neutralising, and adding $AgNO_3$.

Manchot, W. *et al, Chem. Ber.*, 1930, **63**, 1226 (*synth*)
Manchot, W. *et al, Z. Anorg. Allg. Chem.*, 1933, **212**, 109 (*synth*)
Mercer, E.E. *et al, Inorg. Chem.*, 1966, **5**, 1881 (*ir*)
Durig, J.R. *et al, Spectrochim. Acta*, 1966, **22**, 1091 (*ir*)
Buran, E.J. *et al, Chem. Ber.*, 1969, **102**, 3915 (*reaction*)
Buran, E.J. *et al, Z. Anorg. Allg. Chem.*, 1969, **370**, 283 (*ir, uv*)
Claussen, C.A. *et al, J. Am. Chem. Soc.*, 1970, **92**, 7482 (*mössbauer*)
Polzel, W. *et al, Z. Phys.*, 1970, **240**, 306 (*mössbauer*)
Greatrex, R. *et al, J. Chem. Soc. A*, 1971, 1873 (*mössbauer*)
Ivanova, N.V. *et al, Koord. Khim.*, 1975, **1**, 697 (*theory*)
Nikol'skii, A.B. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1976, **231**, 622 (*ir, reaction*)
Gustavsen, D. *et al, Inorg. Chim. Acta*, 1977, **21**, 119 (*synth, uv*)
Nikol'skii, A.B. *et al, Zh. Fiz. Khim.*, 1977, **51**, 1822; *CA*, 1977, **87**, 126480 (*NO exchange*)
Lie, S.K. *et al, Chem. Phys. Lett.*, 1978, **55**, 347 (*mössbauer*)
Nikol'skii, A.B. *et al, Koord. Khim.*, 1979, **5**, 1851 (*synth*)
Nikol'skii, A.B. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1980, **250**, 902 (*photochem*)
Nikol'skii, A.B. *et al, Koord. Khim.*, 1983, **9**, 946 (*photochem*)
Ivanova, N.V. *et al, Teor. Eksp. Khim.*, 1983, **19**, 607 (*uv*)
Mazalov, L.N. *et al, Zh. Strukt. Khim.*, 1987, **28**, 39 (*theory*)
Butler, A.R. *et al, Inorg. Chim. Acta*, 1988, **146**, 187 (*struct, reactions*)

$C_5N_4ORuS_3^{2\ominus}$ IC-004846

(Nitrosyl)pentakis(thiocyanato-*N*)ruthenate(2−), 9CI
Pentaisothiocyanato(nitrosyl)ruthenate(2−)
[40214-87-7]

$[Ru(NO)(NCS)_5]^{2\ominus}$ (C_{4v})

M 421.4 (ion)
Prep. by treating $[Ru(NO)Cl_5]^{2\ominus}$ with an excess of $[SCN]^{\ominus}$. V. sol. H_2O.
Di-K salt: Red-brown solid.
Di-Rb salt: Red-brown solid.
Bis-benzyltriphenylphosphonium salt: Red-brown solid.

Howarth, D.W. *et al, J. Chem. Soc.*, 1964, 3335 (*synth, uv, N-14 nmr*)
Bancroft, G.M. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2643 (*mössbauer*)
Nikol'skii, A.B. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1980, **250**, 902 (*photochem*)

$C_5N_4OS_3Tc^{2\ominus}$ IC-004847

Nitrosylpentakis(thiocyanato-*N*)technetate(2−), 11CI
Pentaisothiocyanatonitrosyltechnetate(II)(2−)

$[Tc(NO)(NCS)_5]^{2\ominus}$

M 419.3 (ion)
Synth. by reduction of $TcO_4^{\ominus}$ in DMF in presence of NH_2OH and $NCS^{\ominus}$, or from reaction of $[Tc(NO)Br_4]^{\ominus}$ with $NCS^{\ominus}$ in MeOH. Reduced to rust-coloured $Tc(NO)(NCS)_5^{3\ominus}$ by N_2H_4, or electrochemically.
Bis-Ph_4As salt: [91356-66-0].
Deep blue cryst. (CH_2Cl_2/C_6H_6). Mp 304-306°.

Orvig, C. *et al, J. Labelled Compd. Radiopharm.*, 1981, **18**, 148 (*synth, ir, conductivity*)
Jones, A.G. *et al, Int. J. Appl. Radiat. Isot.*, 1982, **33**, 867 (*synth, electrochem*)
Baldas, J. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 827 (*synth, ir, esr*)
Kirmse, R. *et al, Z. Anorg. Allg. Chem.*, 1984, **518**, 210 (*esr*)

$C_5N_4OV^{3\ominus}$ IC-004848

Pentakis(cyano-*C*)nitrosylvanadate(3−), 11CI
Pentacyanonitrosylvanadate(3−), 8CI
[36583-32-1]

$[V(NO)(CN)_5]^{3\ominus}$

M 211.0 (ion)
Octahedral with non-linear V—N—O moiety.
Tri-K salt: [23336-32-5].
Synth. by dissolving $[NH_4]VO_3$ in aq. KOH, adding excess KCN and $[NH_3OH]Cl$. Orange solid $+2H_2O$ (H_2O). The anhydrous salt is also known. The dihydrate was previously reported to be a monhydrate.
[37450-82-1]

Griffith, W.P. *et al, J. Chem. Soc. A*, 1959, 1632 (*synth*)
Jagner, S. *et al, Acta Chem. Scand.*, 1970, **24**, 1988 (*synth, ir, cryst struct*)
Folkesson, B., *Acta Chem. Scand., Ser. A*, 1974, **28**, 491 (*ir, esca*)

$C_5N_4O_2Rh^{3\ominus}$ IC-004849

Pentakis(cyano-*C*)nitritorhodate(*III*)(3−)
Nitropentacyanorhodate(III)(3−)

$[Rh(CN)_5(NO_2)]^{3\ominus}$

M 278.9 (ion)
Tri-K salt: Synth. from $RhCl_3.3H_2O$, KCN, K/Hg and NO. White microcryst.

Lawson, D.N. *et al, J. Chem. Soc. A*, 1966, 52 (*synth, ir*)

$C_5N_4OsS_6^{2\ominus}$ IC-004850

Pentakis(thiocyanato-*N*)thionitrosylosmate(2−)
Pentaisothiocyanato(thionitrosyl)osmate(2−)
[82867-79-6]

$[Os(NS)(NCS)_5]^{2\ominus}$ (C_{4v})

M 526.6 (ion)
Bis-Ph_4P salt: [82867-80-9].
Synth. from $[Ph_4P][OsNCl_4]$ with $[Ph_4P][NCS]$ in aq. Me_2CO. Brown-green hexagonal plates(MeCN). Ir ν_{SCS} 2125sh, 2080s, 2050s, ν_{OsNS} 1270s cm^{-1}.

Wright, M.J. *et al, Transition Met. Chem.*, 1982, **7**, 53 (*synth, ir*)

$C_5N_4Re^{3\ominus}$ IC-004851

Pentacyanonitridorhenate(*V*)(3−)

$[N{\equiv}Re(CN)_5]^{3\ominus}$

M 330.3 (ion)
Tri-K salt: [25685-10-3].

Synth. from $K_2[ReN(CN)_4]H_2O$ and KCN in H_2O. Yellow microcryst. (MeOH aq.). Ir $\nu_{Re\equiv N}$ 1035 cm^{-1} (solid).

Johnson, N.P., *J. Chem. Soc. A*, 1969, 1843 (*synth, ir, uv*)

$C_5N_4ReS_5^{2\ominus}$ IC-004852

Nitridopentakis(thiocyanato-*N*)rhenate(*VI*)(2−), 10CI
Pentaisothiocyanato(nitrido)rhenate(VI)(2−)

$[N{\equiv}Re(NCS)_5]^{2\ominus}$

M 490.6 (ion)
Distorted octahedral geometry. Interatomic distances: Re≡N 165.7, Re—N 199.7-205.0 pm.
Bis-Ph_4As salt: [68148-82-3].
Synth. from $AsPh_4[ReNCl_4]$, $AsPh_4NCS$ and KNCS in MeOH. Deep red plates ($CHCl_3$).

Currondo, M.A.A.F. de C.T. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 844 (*synth, cryst struct*)

C_5O_5 IC-004853

1,2,3,4-Pentatetraene-1,5-dione, 11CI
Carbon suboxide (C_5O_2)
[5179-36-1]

O=C=C=C=C=C=O

M 92.0
Formed from 2,4,6-tridiazacyclohexane-1,3,5-trione + hν neat or in Ar matrix at 12K. Yellow solid, dec. at ~ −90°.

Maier, G. *et al, Angew. Chem., Int. Ed. Engl.*, 1988, **27**, 566 (*synth, cmr, ir, uv*)

C_5O_5Os IC-004854

Pentacarbonylosmium
Osmium carbonyl, 9CI. Osmium pentacarbonyl
[16406-49-8]

$Os(CO)_5$

M 330.2
Synth. from $Os_3(CO)_{12}$ and CO (200 atm.) at 280-290°. Colourless to pale-yellow cryst., melting to mobile yellow liq. Sol. common org. solvs. Mp 2-2.5°. Ir ν_{CO} 2035, 1993 cm^{-1}. Cmr 182.6 ppm ($CDCl_3$).

Rushman, P. *et al, Organometallics*, 1983, **2**, 693 (*synth, ir, cmr*)
Huang, J. *et al, Organometallics*, 1988, **7**, 2049 (*struct, ed*)
Shen, J. *et al, Inorg. Chem.*, 1989, **28**, 4304 (*kinetics*)
Shen, J. *et al, Organometallics*, 1989, **8**, 2144 (*use, kinetics*)
Ingalls, *et al, J. Am. Chem. Soc.*, 1990, **112**, 639 (*ir*)

$C_5O_5Re^{\ominus}$ IC-004855

Pentacarbonylrhenate(1−), 10CI, 9CI
[14971-38-1]

$[Re(CO)_5]^{\ominus}$

M 326.2 (ion)
Salts generally prepd. and used *in situ* due to extreme sensitivity to air and moisture.
Na salt: [33634-75-2].
Synth. from $Re_2(CO)_{10}$ + Na/Hg. Yellow-green soln. in THF. Ir ν_{CO} 1917, 1862 cm^{-1} (MeCN).
K salt: [63139-42-4].
Moisture-sensitive.

[35725-77-0]

Hieber, W. *et al, Chem. Ber.*, 1960, **93**, 901 (*synth*)
Moore, E.J. *et al, J. Am. Chem. Soc.*, 1986, **108**, 2257 (*ir*)

C_5O_5Ru IC-004856

Pentacarbonylruthenium
Ruthenium carbonyl ($Ru(CO)_5$). Ruthenium pentacarbonyl
[16406-48-7]

$Ru(CO)_5$

M 241.1
Trigonal bipyramidal. Synth. by high pressure carbonylation of $Ru_3(CO)_{12}$, Ru, RuI_3, RuS_2 or $Ru(acac)_3$, or photochemical degradation of $Ru_3(CO)_{12}$ in heptane under CO. Invaluable synthetic reagent. Colourless liq.; readily dec. at r.t. (or in sunlight or on gentle heating), turning yellow, evolving CO and depositing $Ru_3(CO)_{12}$. Sol. EtOH, C_6H_6, $CHCl_3$, hydrocarbons; insol. H_2O. Mp −22°, Mp −17° to −16°. ΔH_f° −1054 kJ mol^{-1}. Ir ν_{CO} 2035, 1999 cm^{-1} (heptane).

Manchot, W. *et al, Z. Anorg. Allg. Chem.*, 1936, **226**, 385 (*synth, props*)
Calderazzo, F. *et al, Inorg. Chem.*, 1967, **6**, 1220 (*synth, ir, reactions*)
Deeming, A.J. *et al, J. Chem. Soc. A*, 1970, 2967 (*protonation*)
Piacenti, F. *et al, Inorg. Chem.*, 1971, **10**, 2759 (*synth*)
Whyman, R., *J. Organomet. Chem.*, 1973, **56**, 339 (*synth, ir, reactions*)
Johnson, B.F.G. *et al, J. Organomet. Chem.*, 1974, **67**, C75 (*synth*)
Moss, J.R. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 95 (*synth, ir*)
Behrens, R.G., *J. Less-Common Met.*, 1977, **56**, 55 (*thermodyn*)
Tyler, D.R. *et al, J. Am. Chem. Soc.*, 1978, **100**, 7888 (*uv*)
Hug, R. *et al, Inorg. Chim. Acta*, 1980, **38**, 121 (*reactions*)
Yarrow, P. *et al, J. Organomet. Chem.*, 1981, **214**, 115 (*protonation*)
Rushman, P. *et al, Organometallics*, 1983, **2**, 693 (*synth, ir, cmr*)
Seddon, E.A. *et al, The Chemistry of Ruthenium*, Elsevier, Amsterdam, 1984, 927 (*ren, synth, reactions*)

$C_5O_5Tc^{\ominus}$ IC-004857

Pentacarbonyltechnetate(1−)

$[Tc(CO)_5]^{\ominus}$

M 238.9 (ion)
Rare example of technetium in oxidation state −1; anion of $HTc(CO)_5$.

Hileman, J.C. *et al, Inorg. Chem.*, 1962, **1**, 933.

$C_5O_{15}Th^{6\ominus}$ IC-004858

Pentakis(carbonato(2−)-*O,O'*)thorate(6−)
Pentacarbonatothorate(IV)(6−)

$[Th(CO_3)_5]^{6\ominus}$

M 532.0 (ion)
10-Coord. with bicapped square antiprismatic struct. (guanidinium and sodium salts).
Hexa-Na salt: [12388-47-9]
$C_5Na_6O_{15}Th$ M 670.0
Large colourless prisms + $12H_2O$. Sol. H_2O.
Hexa-K salt:
$C_5K_6O_{15}Th$ M 766.6
Colourless prisms + $10H_2O$. Sol. H_2O.
Hexakis-guanidinium salt: [12384-93-1]
Colourless cubic cryst. + $4H_2O$. Sol. H_2O. Mp >150° dec. Slowly effloresces in air. H_2O lost at 50-80°.
Bis-hexaamminecobalt(3+) salt: [41875-80-5]
$C_5H_{36}Co_2N_{12}O_{15}Th$ M 854.3

Affords quantitive pptn. of Th. Ruby-red to orange solid + $10H_2O$. Insol. H_2O, sol. dil. HCl. Mp *ca.* 200° dec. Efflorescent.

Cleve, P.T., *Bull. Soc. Chim. Fr.*, 1874, 115 (*synth*)
Rosenheim, A. *et al*, *Z. Anorg. Allg. Chem.*, 1903, **35**, 424; 1932, **206**, 31 (*synth*)
Canneri, G., *Gazz. Chim. Ital.*, 1925, **55**, 39 (*synth*)
Chernyaev, I.I. *et al*, *Zh. Neorg. Khim.*, 1958, **3**, 2671; 1961, **6**, 587, 809; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1961, **6**, 298, 413.
Kharitonov, Yu.Ya. *et al*, *Zh. Neorg. Khim.*, 1969, **14**, 2761; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 1453 (*synth, ir*)
Ueno, K. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 3817 (*synth*)
Dervin, J. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 2634, 2930.
Voloitis, S. *et al*, *Rev. Chim. Miner.*, 1977, **14**, 441 (*cryst struct*)

$C_6AlF_9O_6$ IC-004859

Aluminium trifluoroacetate
Aluminium tris(trifluoroacetate)

$Al(OOCCF_3)_3$

M 366.0
Synth. from Al/Hg or $AlCl_3$ + F_3CCOOH. White cryst. (H_2O + $(CF_3CO)_2O$). Spar. sol. F_3CCOOH. Complexes with 3Py, 3DMF, 3DMSO, 3THF also descr.

Hara, R. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 4285.
U.S. Pat., 2 882 289, (1959); *CA*, **53**, 22883.
Sartori, P. *et al*, *J. Fluorine Chem.*, 1971, **1**, 463 (*synth, props, complexes*)
Garner, C.D. *et al*, *Adv. Inorg. Chem. Radiochem.*, 1975, **17**, 1 (*rev*)

$C_6AlO_{12}^{3\ominus}$ IC-004860

Tris(oxalato)aluminate(3−)
Tris[ethanedioato(2−)-O,O']aluminate(3−)
[15226-56-9]

$[Al(C_2O_4)_3]^{3\ominus}$

M 291.0 (ion)
Log $\beta \sim 15$.
Tri-K salt, trihydrate: [15242-51-0].
Synth. from Al, KOH and $H_2C_2O_4$. Colourless cryst. (H_2O). Forms mixed cryst. with $K_3[M(C_2O_4)_3].3H_2O$ (M = Cr or Fe).

Inorg. Synth., 1939, **1**, 34 (*synth*)
Palmer, W.G., *Experimental Inorganic Chemistry*, Cambridge, 1954, 213 (*synth*)
Rangarajan, G. *et al*, *J. Phys. Chem.*, 1968, **49**, 5336 (*pmr*)
Zolotukin, V.K. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 367 (*potent. titrations*)
Haraguchi, H. *et al*, *J. Phys. Chem.*, 1969, **73**, 3467 (*Al-27 nmr*)
Dutt, N.K. *et al*, *Indian J. Chem., Sect. A*, 1976, **14**, 491; *CA*, 1978, **88**, 202363 (*tga*)
Gouteron, J., *J. Inorg. Nucl. Chem.*, 1976, **38**, 55 (*ir, raman*)
Jaber, M. *et al*, *Can. J. Chem.*, 1977, **55**, 3689 (*Al-27 nmr, raman*)
Taylor, D., *Aust. J. Chem.*, 1978, **31**, 1455 (*cryst struct*)
Sjöberg, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 2665 (*thermodyn data, Al-27 nmr*)
Smith, R.M. *et al*, *Critical Stability Constants*, Plenum, 2nd Suppl., 1989, **6**.

$C_6Am_2O_{12}$ IC-004861

Americium(*III*) oxalate
Tris(oxalato)diamericium(III). *Tris(ethanedioato) diamericium*(III)

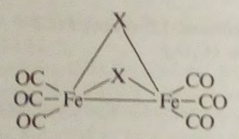
$Am_2(C_2O_4)_3$

M 746.1
Heptahydrate isol.; evidence for tetra- and monohydrates during dehydration of heptahydrate. Anhydrous salt stable to 320°; dec. to AmO_2 over range 320-470°.
Heptahydrate: [16519-58-7].
$C_6H_{14}Am_2O_{19}$ M 872.2
Pink, tan-brown cryst. Loses H_2O on heating >80° in air. Dehydration complete at 230°.
Decahydrate: [18421-70-0].
$C_6H_{20}Am_2O_{22}$ M 926.3
Pink cryst. Isomorphous with Nd, Sm analogues.
[65113-20-4]

Markin, T.L., *J. Inorg. Nucl. Chem.*, 1958, **7**, 290 (*synth, tga*)
Lebedev, I.A. *et al*, *Radiokhimiya*, 1960, **2**, 351; 1962, **4**, 208.
Burney, G.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1967, **3**, 79 (*soly*)
Weigel, F. *et al*, *Inorg. Nucl. Chem. Lett.*, 1967, **3**, 403 (*struct*)

$C_6Br_2Fe_2O_6$ IC-004862

Di-μ-bromohexacarbonyldiiron, 9CI
Bis(tricarbonyliron bromide)
[36190-46-2]



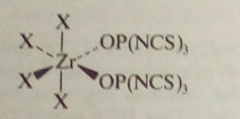
X = Br

M 439.5
Fine dark red needles (pentane). Unstable in soln. Mp 57-59° dec.

Koerner von Gustorf, E. *et al*, *Z. Naturforsch., B*, 1972, **27**, 140 (*synth, ir, uv*)

$C_6Br_4N_6O_2P_2S_6Zr$ IC-004863

Tetrabromobis(phosphoryl isothiocyanate-*O*) zirconium(*IV*), 11CI
Zirconium tetrabromide bis(phosphoryl isothiocyanate). Zirconium(IV) *bromide bis(phosphoryl isothiocyanate)*



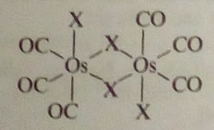
X = Br

M 853.2
Octahedral.
cis-form [85108-12-9]
Synth. from $ZrBr_4$ + $OP(NCS)_3$. White cryst.

Shopenko, V.V. *et al*, *Ukr. Khim. Zh.* (*Russ. Ed.*), 1983, **49**, 3; *CA*, **98**, 154213g (*synth, ir, raman*)

$C_6Br_4O_6Os_2$ IC-004864

Di-μ-bromodibromohexacarbonyldiosmium
Tetrabromohexacarbonyldiosmium
[17731-88-3]



X = Br

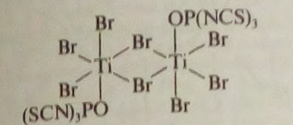
M 868.0

Synth. from $Os_3(CO)_{12}$, BBr_3 and a 3:1 mixture of H_2CO (1 atm.)at 150° for 1 h. Purified by subl. at 190°. Catalyst precursor for hydrogenation reactions. White cryst. (CH_2Cl_2). Mp 315°. Subl. 190° *in vacuo*.
Monomer: Dibromotricarbonylosmium
$C_3Br_2O_3Os$ M 434.0
No separate existence.

Hales, L.A.W. *et al*, *J. Chem. Soc. A*, 1967, 1932 (*synth, ir*)
Choi, H.W. *et al*, *Inorg. Chem.*, 1981, **20**, 2664 (*synth, ms, ir*)

$C_6Br_8N_6O_2P_2S_6Ti_2$ IC-004865

Di-μ-bromohexabromobis(phosphoryl isothiocyanate-*O*) dititanium(*IV*), 11CI
[82474-16-6]



M 1177.4
Octahedral dimer, exact geometry unknown. Synth. by slowly adding a small excess of $PO(NCS)_3$ in CCl_4 to $TiBr_4$ in CCl_4. Moisture-sensitive solid.
Monomer: Tetrabromo(phosphoryl isothiocyanate-O) titanium(IV)
$C_3Br_4N_3OPS_3Ti$ M 588.7
Unknown.

Skopenko, V.V. *et al*, *Dopov. Akad. Nauk Ukr. RSR, Ser. B: Geol., Khim. Biol. Nauki.*, 1982, **44**; *CA*, **97**, 65411g (*synth, ir*)

$C_6CdN_6S_6^{4\ominus}$ IC-004866

Hexakis(thiocyanato-*S*)cadmate(4−)

$[Cd(SCN)_6]^{4\ominus}$

M 460.9 (ion)
Alkali metal salts have been prepd. from $Cd(SCN)_2$ + MSCN in aq. EtOH.
[39584-46-8]

Kharitonov, Yu.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 931 (*synth, ir*)
Tsivadze, A.Yu. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1972, **17**, 1529 (*ir, soln*)

$C_6CdN_6Se_6^{4\ominus}$ IC-004867

Hexakis(selenocyanato)cadmate(4−)

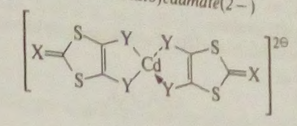
$[Cd(SeCN)_6]^{4\ominus}$

M 742.2 (ion)
Tetra-K salt: [13859-43-3].
Prepd. from KSeCN + $Cd(SeCN)_2$ in Me_2CO.
Colourless rectangular prisms.

Gulub, A.M. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, **7**, 279 (*synth*)

$C_6CdO_2S_8^{2\ominus}$ IC-004868

Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-*S*^{4},*S*^{5}] cadmate(2−), 12CI
Bis(1,3-dithiole-2-one-4,5-dithiolato)cadmate(2−). Bis(2-oxo-1,3-dithiole-4,5-dithiolato)cadmate(2−)



X = O, Y = S

M 473.0 (ion)
Bis-Ph_4As salt: [119797-52-3].
Yellow cryst. Dec. at 224-226°.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **567**, 131 (*synth, ir, cmr*)

$C_6CdS_6Se_4^{2\ominus}$ IC-004869

Bis[4,5-diselenyl-1,3-dithiole-2-thionato(2−)-*Se*,*Se'*] cadmate(2−), 12CI
Bis(2-thioxo-1,3-dithiole-4,5-diselenolato)cadmate(2−)
As Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-*S*^{4},*S*^{5}] cadmate(2−), 12CI, IC-004868 with

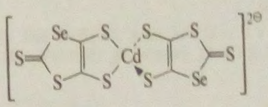
X = S, Y = Se

M 692.7 (ion)
Bis-tetrabutylammonium salt: [120752-54-7].
Red cryst. (Me_2CO/2-propanol). Sol. DMSO. Mp 148-151° dec.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **577**, 206 (*synth, ir, uv-vis, cmr*)
Olk, B. *et al*, *Z. Chem.*, 1989, **29**, 64 (*Se-77 nmr*)

$C_6CdS_8Se_2^{2\ominus}$ IC-004870

Bis(1,3-thiaselenole-2-thione-4,5-dithiolato)cadmate(2−)
Bis[4,5-dimercapto-1,3-thiaselenole-2-thionato(2−)-S^4,*S*^{5}*] cadmate(2−)*



M 598.9 (ion)
Bis-tetrabutylammonium salt: [130744-16-0].
Red cryst. (MeOH). Dec. at 160-163°.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1990, **581**, 59 (*synth, cmr, uv*)

$C_6CdS_{10}^{2\ominus}$ IC-004871

Bis[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-*S*^{4},*S*^{5}] cadmate(2−), 9CI
As Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-*S*^{4},*S*^{5}] cadmate(2−), 12CI, IC-004868 with

X = Y = S

M 505.1 (ion)
Bis-tetrabutylammonium salt: [72688-93-8].
1,1'-Dimethyl-4,4'-bipyridinium(2+) salt: [107769-59-5].
Brown-violet cryst. Mp 207°.

Steimecke, G. *et al*, *Z. Chem.*, 1975, **15**, 28 (*ir*)
Lahner, S. *et al*, *Chem. Ber.*, 1987, **120**, 1011 (*synth, uv-vis*)

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **567**, 131; 1989, **577**, 206 (*synth, ir, cmr, uv-vis*)
Olk, B. *et al*, *Z. Chem.*, 1990, **30**, 105 (*cmr*)

$C_6Ce_2O_{12}$ IC-004872

Cerium(*III*) oxalate
Tris(oxalato)dicerium(III). *Tris(ethanedioato)dicerium*(III)
[7047-99-6]

$Ce_2(C_2O_4)_3$

M 544.2
Decahydrate: [15053-73-3].
$C_6H_{20}Ce_2O_{22}$ M 724.4
μ_{eff} = 2.44μ_B (293K). Presumed 9-coord.; isostructural with Nd analogue. Other hydrates also known.
[139-42-4, 13266-83-6, 15750-47-7, 19511-08-1, 35586-22-2]

Lancaster, F.W. *et al*, *J. Chem. Phys.*, 1951, **19**, 1181; 1952, **20**, 740 (*esr*)
Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth, tga*)
Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Ollendorff, W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Hansson, E., *Acta Chem. Scand.*, 1973, **27**, 823 (*cryst struct*)
Sharov, V.A. *et al*, *Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1979, **5**, 572 (*magnetism*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6Cl_4HfN_6O_2P_2S_6$ IC-004873

Tetrachlorobis(phosphoryl isothiocyanate-*O*)hafnium(*IV*), 11Cl
Hafnium(IV) *chloride bis(phosphoryl isothiocyanate)*

$HfCl_4[OP(NCS)_3]_2$

M 762.7
Octahedral.
cis-form [85165-95-3]
The analogous derivative of $ZrBr_4$ has the same struct.
[74678-35-6]

Skopenko, V.V. *et al*, *Ukr. Khim. Zh.* (*Russ. Ed.*), 1980, **46**, 601; 1983, **49**, 3; *CA*, **93**, 106182w; **98**, 154213g (*synth, ir, raman, struct*)

$C_6Cl_4O_6Os_2$ IC-004874

Hexacarbonyldi-μ-chlorodichlorodiosmium, 9Cl
Hexacarbonyltetrachlorodiosmium
[17633-40-8]
As Di-μ-bromodibromohexacarbonyldiosmium, IC-004864 with

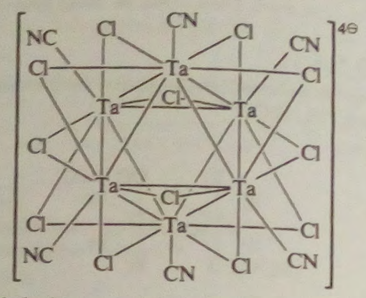
X = Cl

M 690.2
Two isomers known which are prob. structural isomers, not dimorphs.
α-form [22377-51-1]
Colourless cryst. (C_6H_6 or CCl_4). Mp 266°. In $CHCl_3$ soln. isomerises to β-form.
β-form [22377-54-4]
Colourless cryst. ($CHCl_3$). Mp 285°.
Monomer: Tricarbonyldichloroosmium
$C_3Cl_2O_3Os$ M 345.1
No separate existence.

Hales, L.A.W. *et al*, *J. Chem. Soc. A*, 1967, 1932 (*synth, ir*)
Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1969, 372 (*synth, ir, raman*)
Bruce, M.I. *et al*, *J. Chem. Soc. A*, 1969, 987 (*synth, ir*)
Psaro, R. *et al*, *Inorg. Chim. Acta*, 1983, **77**, L255 (*synth*)
Herrmann, W.A. *et al*, *Chem. Ber.*, 1988, **121**, 1907 (*cryst struct, synth*)

$C_6Cl_{12}N_6Ta_6^{4\ominus}$ IC-004875

Dodeca-μ-chlorohexakis(cyano-*C*)hexatantalate(4−), 11Cl



M 1667.2 (ion)
Octahedron of 6 Ta with Cl bridging all edges and a terminal $CN^{\ominus}$ on each Ta.
Tetra-H compd.: [83619-42-5].
Synth. by adding KCN then HCN to a soln. of Ta_6Cl_{14} in MeOH. Brown solid + 12 H_2O (H_2O).

Basson, S.S. *et al*, *Transition Met. Chem.*, 1982, **7**, 207 (*synth, cryst struct*)

$C_6Cm_2O_{12}$ IC-004876

Curium(*III*) oxalate
Tris(oxalato)dicurium(III). *Tris(ethanedioato)dicurium*(III)
[35568-26-4]

$Cm_2(C_2O_4)_3$

M 752.1
Anhydrous complex obtd. by thermal dec. of decahydrate at 280°. On further heating *in vacuo* forms $Cm_2(CO_3)_3$ and Cm_2O_3.
Decahydrate: [21107-06-2].
$C_6H_{20}Cm_2O_{22}$ M 932.3
Pale green cryst. (white). Stable to 60°. Loses H_2O step wise *in vacuo* up to 280°.
▷ Cryst. dec. by α-radiolysis within a few hrs.

Burney, G.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1967, **3**, 79 (*synth*)
Scherer, V. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 1433.

$C_6CoN_5O^{2\ominus}$ IC-004877

Carbonylpentakis(cyano-*C*)cobaltate(*III*)(3−), 11Cl
Carbonylpentacyanocobaltate(III)

$[Co(CN)_5CO]^{2\ominus}$

M 217.0 (ion)
Bis-tetrabutylammonium salt: [89959-52-4].
White cryst. Sol. H_2O.

Palmans, R. *et al*, *Inorg. Chem.*, 1984, **23**, 1792 (*synth, ir, uv*)

$C_6CoN_6^{3\ominus}$ IC-004878

Hexakis(cyano-*C*)cobaltate(*III*)(3−)
Hexacyanocobaltate(III)(*3*−)
[14897-04-2]

$[Co(CN)_6]^{3\ominus}$

M 215.0 (ion)

Pseudo-octahedral complex.
Tri-K salt: [50725-64-9].
$C_6CoK_3N_6$ M 332.3
Synth. from KCN and $Co(CN)_2$, followed by oxidation of the cyanocobaltate(*II*). Yellow cryst. (H_2O). Sol. H_2O; v. sl. sol. liq. NH_3.
Tri-Ag salt:
$C_6Ag_3CoN_6$ M 538.6
White powder.
Tri-H compd.:
$C_6H_3CoN_6$ M 218.0
Obt. by metathesis of tri-K salt. White powder + ½ H_2O.

Inorg. Synth., 1946, **2**, 225 (*synth*)
Ludi, A. *et al*, *Helv. Chim. Acta*, 1967, **50**, 2035 (*synth, powder struct, Ag salt, H compd, thermal dec, ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1684 (*synth, H compd*)
Urushiyama, A. *et al*, *Bunseki Kagaku*, 1981, **30**, 297 (*rev, uv-vis*)
Szargan, R. *et al*, *Inn.-Shell X-Ray Phys. At. Solids*, [Proc. Int. Conf. X-Ray Processes Inn.-Shell Ioniz.], 1981, 717 (*pe*)
Eaton, D.R. *et al*, *J. Phys. Chem.*, 1982, **86**, 1371 (*ir, K salt*)
Potapov, I.A. *et al*, *Kinet. Katal.*, 1982, **23**, 740 (*flash photol, dec*)
Zakharieva-Pencheva, O. *et al*, *Theochem*, 1982, **7**, 241 (*ir, raman*)
Eaton, D.R. *et al*, *Can. J. Chem.*, 1983, **61**, 1524 (*nmr, complexes*)
Au-Yeung, S.C. *et al*, *J. Magn. Reson.*, 1983, **52**, 351 (*Co-59 nmr*)
Korsse, J. *et al*, *Inorg. Chim. Acta*, 1984, **88**, 67 (*electrochem*)

$C_6CoN_6O^{3\ominus}$ IC-004879

(Cyanato-*N*)pentakis(cyano-*C*)cobaltate(*III*)(3−), 9Cl
Isocyanatopentacyanocobaltate(III)(3−)

$[Co(CN)_5NCO]^{3\ominus}$

M 231.0 (ion)
Tri-K salt: [36426-58-1].
Sol. ethylene glycol.

Cohen, M.A. *et al*, *Inorg. Chim. Acta*, 1972, **6**, 188 (*synth, ir, uv*)

$C_6CoN_6S^{3\ominus}$ IC-004880

Pentakis(cyano-*C*)(thiocyanato-*S*)cobaltate(*III*)(3−), 8Cl
Thiocyanatopentacyanocobaltate(III)(*3*−).
Pentacyano(isothiocyanato)cobaltate(III)(*3*−)

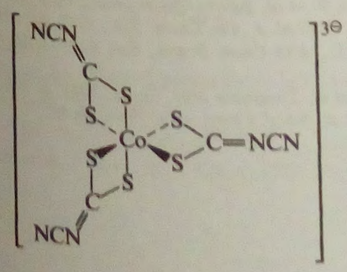
$[Co(CN)_5SCN]^{3\ominus}$

M 247.1 (ion)
Shows linkage isomerism between $[Co(CN)_5NCS]^{3\ominus}$ and $[Co(CN)_5SCN]^{3\ominus}$ species in soln.
Tri-K salt: [19528-41-7].
M 322.3
Yellow orange solid. Sol. H_2O.

Burmeister, J.L. *et al*, *Inorg. Chem.*, 1964, **3**, 919 (*synth, ir*)
Gutterman, D.F. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 3105.

$C_6CoN_6S_6^{3\ominus}$ IC-004881

Tris[*N*-cyanodithiocarbamato(2−)]cobaltate(*III*)(3−), 8Cl



M 407.4 (ion)
Photosensitive.
Tris-diphenyliodonium(1+) salt: [11064-46-3].
Cation and anion react on heating. Green solid. Sol. $MeNO_2$, MeCN, Py, DMF, DMSO. Dec. at 72°.

Ramaswamy, K.K. *et al*, *Inorg. Chem.*, 1970, **9**, 2649 (*synth, ir, props*)

$C_6CoN_6Se^{3\ominus}$ IC-004882

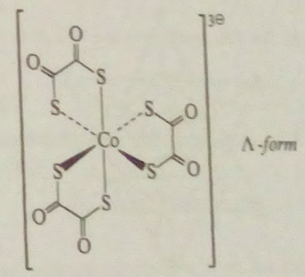
Pentakis(cyano-*C*)selenocyanatocobaltate(*III*)(3−)
$[Co(CN)_5SeCN]^{3\ominus}$

M 293.9 (ion)
N-bonded-form [45113-78-8]
Pentakis(cyano-C)(selenocyanato-N)cobaltate(3−), 9Cl
Pentacyano(isoselenocyanato)cobaltate(III)
Tris-tetrabutylammonium salt: [33848-08-7].
Brown solid. Sol. H_2O, CH_2Cl_2.
Se-bonded-form [57384-14-2]
Pentakis(cyano-C)(selenocyanato-Se)cobaltate(3−), 9Cl
Tri-K salt: [57384-13-1].
Brown solid. Sol. H_2O, CH_2Cl_2, Me_2CO.

Melpolder, J.B. *et al*, *Inorg. Chim. Acta*, 1975, **15**, 91 (*synth, ir, uv*)

$C_6CoO_6S_6^{3\ominus}$ IC-004883

Tris(dithiooxalato)cobaltate(*III*)(3−)
Tris[ethanebis(thioato)(2−)-S,S']cobaltate(3−), 9Cl
[48175-47-9]



M 419.3 (ion)
Λ-form
K, Ba salt: [37604-14-1].
Cryst. + $4H_2O$. Sol. H_2O. $[\alpha]_D$ +700°.
Δ-form
K, Ba salt: Dark brown solid. Sol. H_2O. $[\alpha]_D$ −750°.

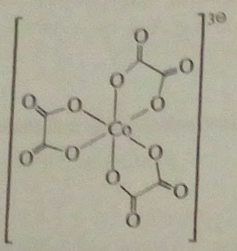
Butler, K.R. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 354 (*cryst struct*)
Dwyer, F.P. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 2335 (*synth, resol*)
Fujita, J. *et al*, *Bull. Chem. Soc. Jpn.*, 1964, **37**, 528 (*ir*)

$C_6CoO_{12}^{3\ominus}$ IC-004884

Tris(oxalato)cobaltate(*III*)(3−)

Tris[ethanedioato(2−)-O,O′]cobaltate(III)(*3−*), *10CI*

[15053-34-6]



M 322.9 (ion)

Subject of studies of kinetics of redox reactions, including with metalloproteins.

Tri-K salt: [15275-08-8].

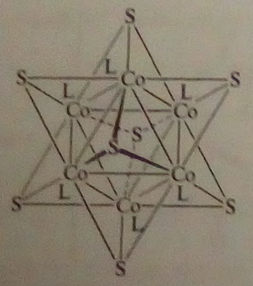
Deep green cryst. + $3H_2O$. Sol. H_2O.

Palmer, W.G., *Experimental Inorganic Chemistry*, Cambridge Univ. Press, 1954, 550 (*synth*)
Hancock, R.D. *et al*, *J. Mol. Struct.*, 1970, **6**, 441 (*ir, raman*)
Butler, K.R. *et al*, *J. Chem. Soc. A*, 1971, 565 (*cryst struct*)
Holwerda, R.A., *J. Am. Chem. Soc.*, 1980, **102**, 1142 (*kinetics*)

$C_6Co_6O_6S_8$ IC-004885

Hexacarbonylocta-μ_3-thioxohexacobalt

Hexacarbonyloctasulfidohexacobalt



L = CO

M 778.1

Octahedron of Co_6 encapsulated in S_8 cube. Co—Co 288.1; Co—S_{av} 216 pm. A 98 electron complex. Mod. air-stable green cryst. + $3S_8$.

Gervasio, G. *et al*, *Inorg. Chim. Acta*, 1984, **83**, L9 (*synth, ir, cryst struct*)

$C_6CrF_9O_8^{\ominus}$ IC-004886

Dioxotris(trifluoroacetato)chromate(*VI*)(1−)

$CrO_2(OOCCF_3)_3^{\ominus}$

M 423.0 (ion)

K salt: [33938-15-7].

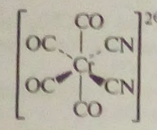
Heat- and light- unstable red brown solid. Easily hydrol.

NH_4 salt: [33071-55-5].

Gerlach, J.N. *et al*, *Inorg. Chem.*, 1971, **10**, 1541 (*synth, ir*)

$C_6CrN_2O_4^{2\ominus}$ IC-004887

Tetracarbonylbis(cyano)chromate(2−)



M 216.0 (ion)

cis-form

Bis(triphenylphosphine)iminium salt: [22142-87-6].

$C_{78}H_{60}CrN_4O_4P_4$ M 1293.2

White, air-stable cryst.

Behrens, H. *et al*, *Z. Anorg. Allg. Chem.*, 1960, **306**, 94.
Behrens, H. *et al*, *Chem. Ber.*, 1964, **97**, 433 (*synth*)
Ruff, J.K., *Inorg. Chem.*, 1969, **8**, 86 (*synth*)

$C_6CrN_6^{6\ominus}$ IC-004888

Hexakis(cyano-*C*)chromate(6−), 11CI, 10CI

Hexacyanochromate(0)(6−)

$[Cr(CN)_6]^{6\ominus}$ (O_h)

M 208.1 (ion)

Synth. by reduction of hexacyanochromate(*III*) or (*II*) by alkali metal in liq. NH_3.

Hexa-Na salt: [79346-55-7].

$C_6CrN_6Na_6$ M 346.0

V. air-sensitive dark green solid, dihydrate, loses $2H_2O$ at 100° *in vacuo*. Diamagnetic.

Hexa-K salt: [15415-54-0].

$C_6CrK_6N_6$ M 442.6

V. air-sensitive dark green solid, dihydrate, loses $2H_2O$ at 100° *in vacuo*. Diamagnetic.

Eaton, J.P. *et al*, *Transition Met. Chem.*, 1981, **6**, 203 (*synth, ir, powder struct*)
Dodsworth, E.S. *et al*, *Inorg. Chim. Acta*, 1984, **89**, 143 (*reaction*)

$C_6CrN_6^{4\ominus}$ IC-004889

Hexakis(cyano-*C*)chromate(*II*)(4−), 10CI, 9CI

Hexacyanochromate(II)(*4−*)

[23209-09-8]

$[Cr(CN)_6]^{4\ominus}$ (O_h)

M 208.1 (ion)

Careful control of pH is necessary to isolate pure salts of this low-spin anion. Powerful reducing agent.

Tetra-Na salt: [79346-49-9].

Blue air-sensitive solid + $2H_2O$; a decahydrate is also known. Dehydrates at 100° *in vacuo*.

Tetra-K salt: [20740-32-3].

$C_6CrK_4N_6$ M 364.4

Green air-sensitive solid + $2H_2O$. Dehydrates at 100° *in vacuo*.

[62483-39-0, 79358-98-8, 79358-99-9]

Bosch-Arino, F. *et al*, *Inform. Quim. Anal.*, 1972, **26**, 231, 254.
Espenson, J.H. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5709.
Lungström, E., *Acta Chem. Scand., Ser. A*, 1977, **31**, 104 (*cryst struct*)
Eaton, J.P. *et al*, *Transition Met. Chem.*, 1981, **6**, 203 (*synth, ir, uv*)
Korsse, J. *et al*, *Inorg. Chim. Acta*, 1984, **88**, 67.

$C_6CrN_6^{3\ominus}$ IC-004890

Hexakis(cyano-*C*)chromate(3−), 11CI, 10CI, 9CI, 8CI

Hexacyanochromate(III)

[14875-14-0]

$[Cr(CN)_6]^{3\ominus}$ (O_h)

M 208.1 (ion)

Kinetically inert, octahedral complex, many salts known. Cr—C 200 to 210 pm; C—N 112 to 119 pm. Undergoes slow aquation to give $[Cr(OH_2)_6]^{3\oplus}$.

Tri-K salt: [13601-11-1].

Synth. from aq. $Cr(OAc)_3$ and KCN. Light-sensitive pale yellow cryst. (H_2O or aq. MeOH). V. sol. H_2O, slow dec., aided by heat and light; insol. alcohols. μ_{eff} = 3.87μ_B (298K).

Cs, Mn(II) *salt:* [82990-00-9].

$C_6CrCsMnN_6$ M 395.9

Synth. from $Cs_3Cr(CN)_6$ and $MnCl_2$ in H_2O. Yellow cryst. + $1H_2O$. Fcc struct. Contains ordered Cr(*III*)—CN—Cr(*II*) arrangement with high spin Mn(*II*). Ferrimagnetic, T_N 90K. Superexchange intections occur via CN bridges.

Hexaamminechromium(*3+*) *salt:* [23540-70-7].

$C_6H_{18}Cr_2N_{12}$ M 362.2

Yellow solid.

Tris(1,2-ethanediamine-N,N′)chromium(*3+*) *salt 1:1:* [55782-98-4].

$C_{12}H_{24}Cr_2N_{12}$ M 440.3

Yellow solid + $2H_2O$.

Hexakis(urea-O)chromium(*3+*) *salt:* [23540-67-2].

$C_{12}H_{24}Cr_2N_{18}O_6$ M 620.4

Synth. from aq. $[Cr(urea)_6]Cl_3$ and $K_3[Cr(CN)_6]$. Light green cryst.

Iron(*2+*) *salt* (*2:3*): [14123-10-5].

$C_{12}Cr_2Fe_3N_{12}$ M 583.7

Synth. from $K_3Cr(CN)_6$ + $Fe^{2\oplus}$ salts. Light brown to orange powder. Shows linkage isomerism.

[20558-40-1, 20792-64-7, 23540-71-8]

Brown, D.B. *et al*, *Inorg. Chem.*, 1968, **7**, 77 (*synth, isom, Fe salt*)
Schläfer, H.L. *et al*, *Inorg. Chem.*, 1969, **8**, 1137.
Schläfer, H.L. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1971, **75**, 878 (*synth, uv*)
Jeftic, L. *et al*, *J. Phys. Chem.*, 1971, **75**, 2381 (*aquation*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1514 (*synth, K salt*)
Figgis, B.N. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 504 (*cryst struct*)
Griebler, W.-D. *et al*, *Z. Naturforsch., B*, 1982, **37**, 832 (*synth, struct, ir, magnetism, CsMn salt*)
Figgis, B.N. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 1587 (*cryst struct*)
Carlin, R.L. *et al*, *Inorg. Chem.*, 1983, **22**, 2832 (*synth, magnetism*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 773 (*rev*)

$C_6CrN_6O_6^{3\ominus}$ IC-004891

Hexakis(cyanato-*N*)chromate(*III*)(3−), 10CI, 9CI

Hexaisocyanatochromate(III)(*3−*)

$[Cr(NCO)_6]^{3\ominus}$

M 304.0 (ion)

Octahedral anion. Ligand probably *N* bonded.

Tris-Ph_4As salt: [38427-00-8].

Green cryst. μ_{eff} = 3.77μ_B (298K).

Bailey, R.A. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 2935 (*synth, uv-vis, ir*)

$C_6CrN_6S_6^{3\ominus}$ IC-004892

Hexakis(thiocyanato-*N*)chromate(*III*)(3−), 10CI

[15276-09-2]

$[Cr(NCS)_6]^{3\ominus}$ (O_h)

M 400.4 (ion)

Useful starting material. V. many salts known.

Tri-K salt: [14282-33-8].

$C_6CrK_3N_6S_6$ M 517.7

Red cryst. (EtOH). V. sol. H_2O, EtOH. Forms a tetrahydrate.

Tris-Et_4N salt: [14837-72-0].

Obt. from $[Et_4N]Br$, $CrCl_3.6H_2O$ and KSCN. Cryst. (Me_2CO). Ir ν_{CN} 2078s cm^{-1}.

Sabatini, A. *et al*, *Inorg. Chem.*, 1965, **4**, 959 (*synth, ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1515 (*synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 837 (*rev*)

$C_6CrN_6Se_6^{3\ominus}$ IC-004893

Hexakis(selenocyanato-*N*)chromate(*III*)(3−), 9CI

[45227-07-4]

$[Cr(NCSe)_6]^{3\ominus}$ (O_h)

M 681.8 (ion)

Tri-K salt: [22764-63-2].

Hygroscopic; purif. by column chromatog. Sol. MeCN. Characterised spectroscopically.

Tris-tetrabutylammonium salt: [57146-71-1].

Solid.

Botar, A. *et al*, *Z. Anorg. Allg. Chem.*, 1975, **417**, 89 (*synth, ir, uv-vis*)

C_6CrO_5S IC-004894

(Carbonothioyl)pentacarbonylchromium, 9CI

[50358-90-2]

$(OC)_5CrCS$ (C_{4v})

M 236.1

Air- and moisture-stable yellow cryst. Sol. hexane.

Angelici, R.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 7516 (*synth*)
Lichtenberger, D.L. *et al*, *Inorg. Chem.*, 1976, **15**, 2015 (*uv*)
Poliakoff, M. *et al*, *Inorg. Chem.*, 1976, **15**, 2022.
Butler, I.S. *et al*, *Inorg. Chem.*, 1976, **15**, 2602 (*ir*)
Butler, I.S. *et al*, *J. Organomet. Chem.*, 1977, **132**, C1 (*synth*)
Saillard, J.Y. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3318 (*cryst struct*)

C_6CrO_5Se IC-004895

(Carbonoselenoyl)pentacarbonylchromium, 10CI

[63356-87-6]

$(OC)_5CrCSe$ (C_{4v})

M 283.0

Highly volatile, air-stable deep-yellow cryst.

Butler, I.S. *et al*, *J. Organomet. Chem.*, 1977, **132**, C1 (*synth*)
Butler, I.S. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **446**, 17.
Butler, I.S. *et al*, *Inorg. Chim. Acta*, 1979, **32**, 113 (*pe*)
Wilkinson, J.R. *et al*, *J. Organomet. Chem.*, 1979, **179**, 159 (*mwr*)
Plowman, K.R. *et al*, *Inorg. Chem.*, 1981, **20**, 2553 (*ir*)
English, A.M. *et al*, *J. Organomet. Chem.*, 1981, **205**, 177 (*synth*)

C_6CrO_6 IC-004896

Hexacarbonylchromium

Chromium carbonyl ($Cr(CO)_6$), *10CI, 9CI, 8CI. Chromium hexacarbonyl*

[13007-92-6]

$Cr(CO)_6$ (O_h)

M 220.0

Catalyst for hydrogenation, isomerisation, water gas shift reaction and alkylation of aromatic hydrocarbons. Colourless cryst. (methylcyclohexane or by subl.). Sl. sol. CCl_4, insol. H_2O, EtOH, Et_2O. Mp 152-155°. Lower carbonyls $Cr(CO)_n$ (n = 5-1) have been isolated e.g. by matrix isolation as unstable species.

▷ Explodes at 210°. GB5075000.

[25875-16-5, 25941-09-7, 53042-53-8, 53108-98-8, 53108-99-9, 53109-00-5, 53109-01-6, 53109-02-7, 53109-11-8, 53109-12-9, 58167-58-1]

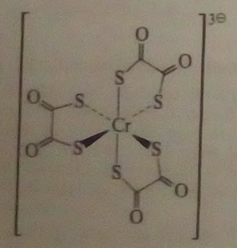
Podall, H.E. *et al, J. Am. Chem. Soc.*, 1961, **83**, 2057 (*synth*)
Whitaker, A. *et al, Acta Crystallogr.*, 1967, **23**, 977 (*cryst struct*)
Rieke, R. *et al, J. Org. Chem.*, 1974, **76**, C19 (*synth*)
Jost, A. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2649 (*nd*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 142; **6**, 125; **7**, 71; **8**, 110; **9**, 117; **10**, 100; **11**, 131 (*uses*)
Bodner, G.M., *Inorg. Chem.*, 1975, **14**, 2694 (*cmr*)
Michels, G.D. *et al, Inorg. Chem.*, 1980, **19**, 479.
Calhorda, M.J. *et al, J. Organomet. Chem.*, 1984, **262**, 305 (*thermochem*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 1852 (*haz*)

$C_6CrO_6S_6^{3\ominus}$ IC-004897

Tris(dithiooxalato)chromate(*III*)

Tris[ethanedithioato(2−)-S,S′]chromate(III)(3−).
Tris[ethanebis(thioato)(2−)-S,S′]chromate(III),(3−), *10CI, 9CI*

[19323-32-1]



M 412.4 (ion)

Δ-config. assigned to (+)-form ion.

K, Ca salt: Solid + $6H_2O$.

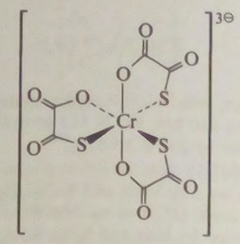
Tris[triphenyl(phenylmethyl)phosphonium] salt: [68249-71-8]. Green-brown solid ($CHCl_3$/MeOH).

Hidaka, J. *et al, Inorg. Chem.*, 1964, **3**, 1724 (*cd, ir, uv-vis*)
Coucouvanis, D. *et al, J. Am. Chem. Soc.*, 1973, **95**, 5556 (*synth, props*)
Vella, P. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 613 (*electrochem, synth*)

$C_6CrO_9S_3^{3\ominus}$ IC-004898

Tris(monothiooxalato)chromate(*III*)(3−)

Tris[(thiocarboxy)formato(2−)]chromate(III)(3−), *10CI*



M 364.2 (ion)

Detailed config. not reported.

Tris-benzyltriphenylphosphonium salt: [64460-36-2]. Green cryst. + $1CH_2Cl_2$ (CH_2Cl_2/Et_2O). Mp 144-145°. μ_{eff} = 3.90μ_B (294K).

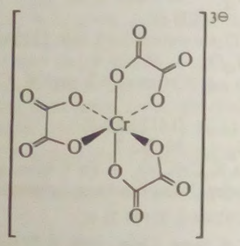
Leitheiser, M. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 811 (*synth, uv-vis, magnetism, ir*)

$C_6CrO_{12}^{3\ominus}$ IC-004899

Tris(oxalato)chromate(*III*)(3−)

Tris[ethanedioato(2−)-O,O′]chromate(III)(3−), *10CI*

[15054-01-0]



M 316.0 (ion)

Distorted octahedral anion.

Tri-K salt: [14217-01-7]. Dichroic cryst. + $3H_2O$: green blue by transmitted light, magenta by reflection. V. sol. H_2O.

Tri-NH_4 salt: Dark blue plates + $2H_2O$.

[15275-09-9]

van Niekerk, J.N. *et al, Acta Crystallogr.*, 1952, **5**, 499 (*cryst struct, NH_4 salt*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1514 (*synth*)
Taylor, D., *Aust. J. Chem.*, 1978, **31**, 1455 (*cryst struct, K salt*)
Inorg. Synth., 1979, **19**, 127 (*synth*)

$C_6Cu_4N_6^{2\ominus}$ IC-004900

Bis[[μ-(cyano-*C*:*N*)]bis(cyano-*C*)dicuprate(1−)], 11CI

$[[Cu_4(CN)_6]^{2\ominus}]_n$

M 410.2 (ion)

Polymeric anion of six-membered rings in infinite sheets. Cu is trigonal planar; Cand N disordered over cyano positions.

Tetraamminecopper(2+) salt: [52504-74-2].
$C_6H_{12}Cu_5N_{10}$ M 541.9
Violet cryst.

[94100-40-0]

Morgan, G.T. *et al, J. Chem. Soc.*, 1926, 2018 (*synth*)

Kello, E. *et al, Z. Anorg. Allg. Chem.*, 1975, **417**, 229 (*synth, ir, uv, cryst struct*)
Koziskova, Z. *et al, Chem. Zvesti*, 1984, **38**, 583 (*cryst struct*)

$C_6Dy_2O_{12}$ IC-004901

Dysprosium(*III*) oxalate

Tris(oxalato)didysprosium(III). *Tris(ethanedioato)didysprosium*(III)

[867-62-9]

$Dy_2(C_2O_4)_3$

M 589.0

Decahydrate: [24670-07-3].
$C_6H_{20}Dy_2O_{22}$ M 769.2
Yellow cryst. μ_{eff} = 10.41μ_B, presumed 9-coord.

[52482-46-9, 58176-69-5]

Wendlandt, W.W., *Anal. Chem.*, 1959, **31**, 408 (*dta*)
Grzymalski, Z. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Ollendorff, W. *et al, Inorg. Nucl. Chem. Lett.*, 1969, **5**, 269 (*struct*)
Hansson, E., *Acta Chem. Scand.*, 1973, **27**, 823 (*synth*)
Sharov, V.A. *et al, Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Fuller, M.J. *et al, J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al, J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6ErN_6S_6^{3\ominus}$ IC-004902

Hexakis(thiocyanato-*N*)erbate(*III*)(3−)

Hexakis(isothiocyanato)erbate(III)(3−)

$[Er(NCS)_6]^{3\ominus}$

M 515.7 (ion)

Octahedral.

Tris-tetrabutylammonium salt: [21315-86-6]. Peach-coloured cryst. Sol. $PhNO_2$, CH_2Cl_2, $MeNO_2$, MeCN, MeOH, EtOH. Mp 170°. Paramagnetic: μ_{eff} = 9.48μ_B. Similar compds. isol. for other Lanthanides. Ir $\nu_{C\equiv N}$ 2090, 2045 cm^{-1} (KBr, nujol).

Martin, J.L. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4493 (*synth, cryst struct*)
Burmeister, J.L. *et al, Inorg. Chim. Acta*, 1969, **3**, 105 (*synth*)
Radonovick, L.J. *et al, Acta Crystallogr., Sect. C*, 1990, **46**, 1618 (*cryst struct*)

$C_6Er_2O_{12}$ IC-004903

Erbium(*III*) oxalate

Tris(oxalato)dierbium(III). *Tris(ethanedioato)dierbium*(III)

[867-63-0]

$Er_2(C_2O_4)_3$

M 598.5

Hexahydrate: [30618-31-6].
$C_6H_{12}Er_2O_{18}$ M 706.6
Pink cryst. Normal hydrate obtd. on cryst. Presumed 8-coord. like Yb analogue.

Decahydrate:
$C_6H_{20}Er_2O_{22}$ M 778.7
Pink cryst. Obtd. on cryst > 50°; presumed 9-coord. like Nd analogue.

Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth, tga*)
Grzymalski, Z. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Watanabe, M. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 3604 (*struct*)
Hansson, E., *Acta Chem. Scand.*, 1973, **27**, 823 (*synth, struct*)
Sharov, V.A. *et al, Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Fuller, M.J. *et al, J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al, J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6EuF_9O_6$ IC-004904

Tris(trifluoroacetato)europium(*III*)

Europium(III) *trifluoroacetate*

[70236-95-2]

$Eu(OOCCF_3)_3$

M 491.0

Forms complexes with crown ethers.

Trihydrate: [94079-71-7].
Prob. dimeric, with 8-coordinate Eu bound to $3H_2O$, 4 bridging O, 1 terminal O. Loses H_2O at 70° *in vacuo*. μ_{eff} = 3.45μ_B.

18-Crown-6 complex (1:1):
$C_{18}H_{24}EuF_9O_{12}$ M 755.3
Hygroscopic. 2:1 deriv. also obt.

Bis(15-crown-5) complex: Hygroscopic cryst.

Singh, M. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 1939 (*synth, magnetism*)
Bünzli, J.C.G. *et al, Inorg. Chim. Acta*, 1985, **110**, 225 (*synth, ir, luminescence, complexes*)

$C_6EuN_6S_6^{3\ominus}$ IC-004905

Hexakis(thiocyanato-*N*)europate(3−)

Hexaisothiocyanatoeuropate(3−)

$[Eu(NCS)_6]^{3\ominus}$

M 500.4 (ion)

Octahedral.

Tris-Et_4N salt: [67481-69-0]. Pale yellow cryst.

Tris-tetrabutylammonium salt: [26395-53-9]. Pale yellow cryst. Sol. MeCN, MeOH, $MeNO_2$, CH_2Cl_2.

Tris-butyltriphenylphosphonium salt: [67270-08-0]. Pale yellow cryst.

Martin, J.L. *et al, J. Am. Chem. Soc.*, 1968, **90**, 4493 (*synth*)
Burmeister, J.L. *et al, Inorg. Chim. Acta*, 1969, **3**, 105 (*synth, ir*)
Bünzli, J.C.G. *et al, Conf. Ser. Inst. Phys.*, 1985, 1978, 115; *CA*, 1978, **89**, 120053 (*luminescence*)
LeMire, A.E. *et al, J. Coord. Chem.*, 1978, **8**, 81 (*nmr*)
de Almeida Santos, R.H. *et al, Quim. Nova*, 1980, **1**, 49 (*cryst struct*)
Matta, O.L. *et al, J. Lumin.*, 1982, **26**, 337 (*luminescence*)
De Azevedo, W.M. *et al, Solid State Commun.*, 1983, **46**, 465 (*luminescence*)

$C_6Eu_2O_{12}$ IC-004906

Europium(*III*) oxalate

Tris(oxalato)dieuropium(III). *Tris(ethanedioato)dieuropium*(III)

[3269-12-3]

$Eu_2(C_2O_4)_3$

M 567.9

Decahydrate: [14175-02-1].
$C_6H_{20}Eu_2O_{22}$ M 748.1
Colourless solid. Loses H_2O on heating. Presumed 9-coord.

[83333-20-4]

Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58; 1959, **31**, 408 (*synth, dta, tga*)

Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Ollendorff, W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Gallagher, P.K. *et al*, *Inorg. Chem.*, 1970, **9**, 215 (*dta, ir, mössbauer*)
Tsaryuk, V.I. *et al*, *Koord. Khim.*, 1977, **3**, 465; *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1977, **3**, 352 (*luminescence*)
Gupta, D.K. *et al*, *Indian J. Pure Appl. Phys.*, 1979, **17**, 546 (*mössbauer*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6F_3MnO_5S$ IC-004907

Pentacarbonyl(trifluoromethanethiolato)manganese, 9CI

[50979-57-2]

$F_3CSMn(CO)_5$

M 296.0
Readily eliminates CO to give di- and trinuclear species. Synth. by photolysis of $Mn_2(CO)_{10}$ with CF_3SSCF_3. Pale-yellow solid; not isol. pure. Ir ν_{CO} 2142w, 2052vs, 2018m cm^{-1}.

Davidson, J.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1957 (*synth, ir, F-19 nmr*)
Grobe, J. *et al*, *J. Fluorine Chem.*, 1978, **11**, 265 (*synth, ir, F-19 nmr*)

$C_6F_3MnO_5Se$ IC-004908

Pentacarbonyl(trifluoromethaneselenolato)manganese, 10CI

[66672-65-9]

$F_3CSeMn(CO)_5$

M 342.9
Synth. from $HMn(CO)_5$ and $CF_3SeSeCF_3$. Yellow oil. Ir ν_{CO} 2128w, 2044vs,br, 2010s cm^{-1}.

Grobe, J. *et al*, *J. Fluorine Chem.*, 1978, **11**, 265 (*synth, ir, F-19 nmr*)

$C_6F_5Xe^{\oplus}$ IC-004909

Pentafluorophenylxenon(*II*)(1+)

$[C_6F_5Xe]^{\oplus}$

M 298.3 (ion)
Fluorotris(pentafluorophenyl)borate:
$C_{24}BF_{21}Xe$ M 829.3
Formed from XeF_2 + $(C_6F_5)_3B$ in MeCN at 0°. Solid, rapidly dec. in H_2O to C_6HF_5. Sol. CH_2Cl_2/MeCN.

Naumann, D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 47, 625 (*synth, cmr, F-19 nmr, Xe-129 nmr, cryst struct*)

$C_6F_9GaO_6$ IC-004910

Gallium(*III*) trifluoroacetate

Gallium tris(trifluoroacetate). Tris(trifluoroacetato)gallium

$Ga(OOCCF_3)_3$

M 408.7
Synth. from $GaCl_3$ + CF_3CO_2H at 70°. White hygroscopic powder. Mp 260° dec. Complexes with 3Py and 3DMF descr.

Sartori, P. *et al*, *J. Fluorine Chem.*, 1971, **1**, 463 (*synth, props*)

$C_6F_9InO_6$ IC-004911

Indium(*III*) trifluoroacetate

Tris(trifluoroacetato)indium

[36554-90-2]

$In(OOCCF_3)_3$

M 453.8
Synth. from In + CF_3COOH. Colourless v. hygroscopic solid. Mp 317° dec. Complexes with 3Py and THF descr. $In(OCOC_3F_7)_3$ also descr.

Sartori, P. *et al*, *J. Fluorine Chem.*, 1972, **1**, 463 (*synth, props*)

$C_6F_9LaO_6$ IC-004912

Lanthanum(*III*) trifluoroacetate

Tris(trifluoroacetato)lanthanum(III)

[70236-92-9]

$(F_3CCOO)_3La$

M 477.9
Hygroscopic, colourless powder. Sol. H_2O.
Trihydrate: [62266-77-7].
$C_6H_6F_9LaO_9$ M 531.9
Colourless cryst. Sol. H_2O. 8-Coord., loses H_2O *in vacuo*. Diamagnetic.
Bis(tetramethylene sulfoxide) complex:
$C_{14}H_{16}F_9LaO_8S_2$ M 686.2
Colourless cryst. 8-Coord. distorted triangular dodecahedron at La. Chain struct.

Roberts, J.E., *J. Am. Chem. Soc.*, 1961, **83**, 1087 (*synth*)
Rillings, K.W. *et al*, *Thermochim. Acta*, 1974, **10**, 285 (*synth, tga, dta, ir*)
Aslanov, L.A. *et al*, *Koord. Khim.*, 1976, **2**, 1674; *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1976, **2**, 1292 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 56 (*rev, bibl*)
Castellano, E.E. *et al*, *Inorg. Chim. Acta*, 1985, **110**, 77 (*synth, cryst struct*)

$C_6F_9NdO_6$ IC-004913

Neodymium(*III*) trifluoroacetate

Tris(trifluoroacetato)neodymium(III)

[29770-44-3]

$(F_3CCOO)_3Nd$

M 483.2
Hygroscopic powder. Sol. H_2O.
Trihydrate: Pink cryst. Sol. H_2O. Loses H_2O *in vacuo* or above 70°. $\mu_{eff} = 3.56\mu_B$.
Bis(tetramethylene sulfoxide) complex: Pink cryst. Dimer, 8-coord. distorted antiprism.

Roberts, J.D., *J. Am. Chem. Soc.*, 1961, **83**, 1087 (*synth, tga*)
Rillings, K.W. *et al*, *Thermochim. Acta*, 1974, **10**, 285 (*synth, ir, dta, tga*)
Singh, M. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1939 (*synth, ir, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 57 (*rev, bibl*)
Castellano, E.E. *et al*, *Inorg. Chim. Acta*, 1985, **110**, 77 (*synth, cryst struct*)

$C_6F_9O_6Pr$ IC-004914

Praseodymium(*III*) trifluoroacetate

Tris(trifluoroacetato)praseodymium(III)

[70236-94-1]

$(F_3CCOO)_3Pr$

M 479.9
Green solid. Dec. ~ 248°.
Trihydrate (dimeric): [55135-12-1].
$C_{12}H_{12}F_{18}O_{18}Pr_2$ M 1068.0
Pale green cryst. Sol. H_2O. Dimeric 8-coord. (distorted sq. antiprismatic coord. at Pr). Loses H_2O on heating. $\mu_{eff} = 5.34\mu_B$.

Hara, R. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 4285 (*synth*)
Rillings, K.W. *et al*, *Thermochim. Acta*, 1974, **10**, 285 (*synth, ir, tga, dta*)
Bone, S.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1544 (*cryst struct*)
Singh, M. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1939 (*synth, ir, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 57 (*rev, bibl*)

$C_6F_9O_6Tl$ IC-004915

Thallium(*III*) trifluoroacetate

TTFA

[23586-53-0]

$Tl(OOCCF_3)_3$

M 543.4
Prepd. by heating a suspension of Tl_2O_3 in CF_3COOH containing 10-20% H_2O. Electophilic thallating agent used in org. synthesis. White solid. H_2O sensitive. Mp >100° dec.

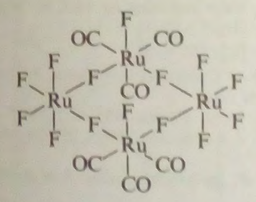
McKillop, A. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 4841 (*synth, use*)
Hsieh, A.T.T. *et al*, *J. Org. Chem.*, 1972, **37**, 2637 (*ms*)
Larock, R.C. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 1900 (*synth*)
Sakae, U., *Synth. Reagents*, 1983, 165 (*rev, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1986, **12**, 481 (*use*)

$C_6F_{14}O_6Ru_4$ IC-004916

***cyclo*-Hexacarbonyltetra-μ-fluorodecafluorotetraruthenium, 9CI**

Bis[tricarbonyldifluororuthenium(II)*-ruthenium*(V) *fluoride]. Hexacarbonyltetradecafluorotetraruthenium*

[59537-02-9]



M 838.3
Prepd. by treating Ru_4F_{20} with CO in flow system at 200°, or by heating $[Ru_3(CO)_{12}]$ with XeF_2 in CCl_2FCF_2Cl at 100°. Air-sensitive solid. $\mu_{eff} = 4.45\mu_B$ per 2Ru atoms.

Hewitt, A.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 579 (*synth, ir, reactions*)

$C_6F_{18}Ge_2Hg$ IC-004917

Bis[tris(trifluoromethyl)germyl]mercury

[82477-25-6]

$(F_3C)_3GeHgGe(CF_3)_3$

M 759.8
Cryst. Mp 135°. $Subl._{0.1}$ 70°. Slow dec. in air. Thermal dec. at 160° with release of mercury. Readily hydrol.

Bochkarev, M.N. *et al*, *J. Organomet. Chem.*, 1982, **229**, C1 (*synth, ir, Hg-199 nmr, F-19 nmr*)
Ermolaev, N.L. *et al*, *Zh. Obshch. Khim.*, 1984, **54**, 96 (*synth*)

$C_6FeN_5O^{3\ominus}$ IC-004918

Carbonylpentakis(cyano-*C*)ferrate(*II*)(3−), 11CI

Carbonylpentacyanoferrate(II)(3−)

[17455-62-8]

$[Fe(CO)(CN)_5]^{3\ominus}$

M 213.9 (ion)
Octahedral anion. Not readily oxidised to an iron(*III*) derivative. Best synth. from $[Fe(CN)_5(NH_3)]^{3\ominus}$ with CO. Alkali metal salts sol. H_2O.
Tri-Na salt: [15418-38-9].
Forms a dihydrate.
Tri-K salt: [26285-25-6].
Synth. from $K_4[Fe(CN)_6]$ + CO under pressure (130-300°). Precursor to Prussian Blue analogue films. Yellow green (H_2O).
Fe(III) *salt:* [70472-77-4].
$C_6Fe_2N_5O$ M 269.7
Prussian Blue analogue.
Tri-H compd.: Carbonylpentacyanoferrous acid
$C_6H_3FeN_5O$ M 216.9
Synth. from Cu(*II*) salt with H_2S, then evaporation. Colourless photosensitive substance (acidic aq. soln.). Sol. H_2O.

[83484-26-8]

Manchot, W. *et al*, *Ber.*, 1912, **45**, 2869 (*synth*)
Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1953, **272**, 32 (*synth*)
Toma, H.E. *et al*, *Inorg. Chim. Acta*, 1979, **33**, L157 (*mössbauer, nmr*)
Inoue, H. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **483**, 75 (*mössbauer*)
Inoue, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 733 (*magnetism, ir, mössbauer, uv-vis*)
Griffith, W.P. *et al*, *Inorg. Chim. Acta*, 1987, **126**, 179 (*ir, nmr*)

$C_6FeN_6^{4\ominus}$ IC-004919

Hexakis(cyano-*C*)ferrate(*II*)(4−), 11CI

Hexacyanoferrate(II)(4−). *Ferrocyanide*

[13408-63-4]

$[Fe(CN)_6]^{4\ominus}$ (O_h)

M 211.9 (ion)
Alkali and alkaline earth (except Ba) salts sol. H_2O; insol. EtOH. Low spin Fe(*II*) but crosses over to high spin at 2×10^5 atm. pressure.
Tetra-K salt: [13943-58-3]. *Potassium ferrocyanide*
$C_6FeK_4N_6$ M 368.3
Pale yellow cryst. + $3H_2O$ (H_2O).
K, Cr(III) *salt: Chromium*(III) *potassium ferrocyanide*
$C_6CrFeKN_6$ M 303.0
Polymeric with Cr—N≡C—Fe linkages.
Di-K, Ni(II) *salt:* [13601-16-6]. *Nickel potassium ferrocyanide*
$C_6FeK_2N_6Ni$ M 348.8
Synth. form $K_4Fe(CN)_6.3H_2O$ + $Ni(NO_3)_2.6H_2O$ + KCl in H_2O.
Fe(III) *salt (3:4):* [14038-43-8]. *Ferric ferrocyanide*
$C_{18}Fe_7N_{18}$ M 859.2
Fe(III) *salt (3:4), tetradecahydrate:* [19611-22-8]. *Prussian blue. Iron blue. Pigment blue 27. Berlin blue. Chinese blue. Hamburg blue. Paris blue*
$C_{18}H_{28}Fe_7N_{18}O_{14}$ M 1111.4

Synth. from $K_4Fe(CN)_6$ in 10*M* HCl with $FeCl_3$. Dye; removes H_2S from flue gases. Blue cubic cryst. (H_2O/diffusing into conc. HCl). Insol. H_2O.

Tetra-H compd.: [17126-47-5]. *Ferrocyanic acid*
$C_6H_4FeN_6$ M 215.9
White powder turning blue in moist air. Sol. H_2O, EtOH. Strong acid; dec. on heating.

Tetra-NH_4 salt: [38670-32-5]. *Tetraammonium ferrocyanide monohydrate*
Solid + $1H_2O$. Heating *in vacuo* to 320° gives a green solid of empirical formula $Fe(CN)_2$.

Weiser, H.B. *et al, J. Phys. Chem.*, 1942, **46**, 99 (*synth, prussian blue*)
Pospelov, V.A. *et al, Zh. Fiz. Khim.*, 1947, **21**, 879 (*struct*)
Shriver, D.F. *et al, Inorg. Chem.*, 1965, **4**, 725 (*synth, ir, uv*)
Ginsberg, A.P. *et al, Inorg. Chem.*, 1965, **4**, 1186 (*ir*)
Shriver, D.F., *Struct. Bonding (Berlin)*, 1966, **1**, 32 (*rev, bibl*)
Pierrot, P.M. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 1685 (*struct*)
Buser, H.J. *et al, J. Chem. Soc., Chem. Commun.*, 1972, 1299 (*cryst struct, prussian blue*)
Hirota, M. *et al, Chem. Lett.*, 1973, 853 (*cmr*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, N.Y., 1976, 103.
Compr. Coord. Chem., Pergamon, Oxford, 1987, **4**, 1204 (*rev, bibl*)

$C_6FeN_6^{3\ominus}$ IC-004920

Hexakis(cyano-*C*)ferrate(*III*)(3−)
Hexacyanoferrate(III)(*3*−). *Ferricyanide*(*3*−)
[13408-62-3]

$[Fe(CN)_6]^{3\ominus}$ (O_h)

M 211.9 (ion)
Fe—C 195 pm. Oxidising agent; $[Fe(CN)_6]^{3\ominus}/[Fe(CN)_6]^{4\ominus}$ E° + 0.36V. Characteristic ir ν_{CN} 2090-2150 cm^{-1}.
▷ Toxic.

Tri-Li salt: [13601-17-7]. *Lithium ferricyanide*
Tri-Na salt: [14217-21-1]. *Sodium ferricyanide*
$C_6FeN_6Na_3$ M 280.9
Ruby-red deliquescent cryst. + $1H_2O$.
Tri-K salt: [13746-66-2]. *Potassium ferricyanide. Red pussate of potash*
$C_6FeK_3N_6$ M 329.2
Synth. by oxidation of $[Fe(CN)_6]^{4\ominus}$ using chlorine. Commercially available. Mild oxidising agent; used in biosensors, analytical reagent. Red cryst., dimorphic. Paramagnetic; μ_{eff} = 2.25μ_B (300K); struct. phase transition at ~130K.
▷ LJ8225000.
Fe(III) *salt:* [14433-93-3]. *Iron*(III) *ferricyanide. Berlin green. Ferric ferricyanide*
$C_6Fe_2N_6$ M 267.8
Fe(II) *salt*(*2:3*)*: Ferrous ferricyanide. Turnbull's blue. Iron blue*
$C_{12}Fe_5N_{12}$ M 591.4
Pigment esp. for blueprints. Deep blue solid.
Tri-H compd.: [17126-46-4]. *Ferricyanic acid*
$C_6H_3FeN_6$ M 214.9
Unstable; strong acid in aq. soln. Brown-yellow. Sol. H_2O, EtOH; insol. Et_2O. Mp 50-60° dec.

Shriver, D.F., *Struct. Bonding (Berlin)*, 1966, **1**, 32 (*bonding, bibl*)
Figgis, B.N. *et al, Proc. R. Soc. London, A*, 1969, **309**, 91 (*magnetism*)
Greenwood, N.N. *et al, Mössbauer Spectroscopy*, Chapman and Hall, 1971 (*mössbauer*)
Vannerberg, N.-G., *Acta Chem. Scand.*, 1972, **26**, 2863 (*struct*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1656 (*H compd*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, London, 1976, 109 (*bibl*)
Inoue, H. *et al, Z. Anorg. Allg. Chem.*, 1981, **483**, 75 (*mössbauer, esca*)
Smith, D.A. *et al, Anal. Chem.*, 1985, **57**, 2361 (*exafs*)
Yoshikawa, S. *et al, J. Biol. Chem.*, 1985, **260**, 3518 (*ir, hemeprotein binding site*)
Morioka, Y. *et al, J. Phys. Soc. Jpn.*, 1985, **54**, 2184 (*struct*)

$C_6FeN_6Pb_2$ IC-004921

Lead(*II*) hexacyanoferrate(*II*)
Lead ferrocyanide. Hexacyanoferrate(*4*−) *lead*(*2*+) *salt*
[14402-61-0]

$Pb_2Fe(CN)_6$

M 626.3
Yellowish-white powder + H_2O. Insol. cold H_2O; sl. sol. H_2SO_4. Loses H_2O at 100°.

Seifer, G.B., *Zh. Neorg. Khim.*, 1959, **4**, 1860; 1963, **8**, 2541 (*synth*)
Rock, P.A. *et al, Inorg. Chem.*, 1964, **3**, 1593.
Seifer, G.B. *et al, Zh. Neorg. Khim.*, 1965, **10**, 1022.
Bellano, A. *et al, Proc. Conf. Appl. Phys. Chem. 2nd*, 1971, **1**, 165.
Tennakone, K., *J. Phys. C*, 1983, **16**, L1193.

$C_6FeN_6S_6^{3\ominus}$ IC-004922

Hexakis(thiocyanato-*N*)ferrate(*III*)(3−), 11Cl
Hexa(*isothiocyanato*)*ferrate*(III)(*3*−)
[45227-67-6]

$[Fe(NCS)_6]^{3\ominus}$ (O_h)

M 404.3 (ion)
Prepd. in non-aq. conditions. Red complexes formed by Fe(*III*) and thiocyanate ions are usually hydrated and blood red colour is due mainly to Pentaaqua(isothiocyanato)iron(*II*)(2+), IC-002638. Catalyst for Ph_3P oxidn.

Tri-K salt: [22949-71-9].
Tris-Me_4N salt: [17499-80-8].
Synth. from $Fe(NO_3)_3.9H_2O$ in EtOH, KNCS in Me_2CO and hot Me_4NNCS in EtOH. Dark green cryst. or red powder. Deep red solns. in alcohols, Me_2CO, nitrobeneze, nitromethane or MeCN. Mp 254°.
Tris-Et_4N salt: [16972-83-1].
Tris-Ph_4P salt: [82139-56-8].
Vogel's Textbook of Quantitative Inorganic Analysis, Longman, 4th Edn., 1954, 741 (*use*)
Forster, D. *et al, Inorg. Chem.*, 1965, **4**, 715 (*ir*)
Forster, D. *et al, J. Chem. Soc.*, 1965, 268 (*uv, magnetism, ir, synth*)
Clark, R.J.H. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 323 (*ir, raman*)
Muller, U., *Acta Crystallogr., Sect. B*, 1977, **33**, 2197 (*cryst struct*)
Folkesson, B. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1982, **26**, 157 (*esca*)

C_6FeN_6Sn IC-004923

Tin(*IV*) ferrocyanide
Tin(IV) *hexakis*(*cyano*-C)*ferrate*(II)(*4*−). *Hexakis*(*cyano*-C)*ferrate*(*4*−) *tin*(*4*+) *salt*
[14239-25-9]

$Sn^{IV}[Fe^{II}(CN)_6]$

M 330.6
Insol. H_2O. Dec. in hot HCl.

Burin, K. *et al, God. Sofii. Univ., Fiz. Mat. Fak.*, 1976, **68**, 133 (*mössbauer*)

Gill, J.S., *J. Radioanal. Chem.*, 1977, **36**, 345 (*ir, mössbauer, synth*)
Bini, A.S. *et al, Italian J. Chem., Sect. A*, 1980, **19**, 165 (*mössbauer*)

$C_6FeN_6Sn_2$ IC-004924

Tin(*II*) ferrocyanide
Tin(II) *hexakis*(*cyano*-C)*ferrate*(II)(*4*−). *Hexakis*(*cyano*-C)*ferrate*(*4*−) *tin*(*2*+) *salt. Stannous ferrocyanide*
[27878-77-9]

$Sn(II)_2Fe(II)(CN)_6$

M 449.3
Synth. from potassium ferrocyanide and a tin salt. White gelatinous mass. Insol. H_2O. Dec. in HCl.
Tetrahydrate: White cryst. Dehydrates *in vacuo* or by heating in a stream of N_2 at 140°. Ir ν 2075vs cm^{-1} (KBr).

Ayers, J.B. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 721 (*synth, props, uv-vis, ir*)
Banchev, Ts. *et al, God. Sofii. Univ., Fiz. Mat. Fak.*, 1974, **66**, 121 (*synth, mössbauer, uv-vis*)
Burin, K. *et al, God. Sofii. Univ., Fiz. Mat. Fak.*, 1976, **68**, 133 (*mössbauer*)
Siebert, H. *et al, Z. Anorg. Allg. Chem.*, 1981, **474**, 96 (*cryst struct*)

$C_6FeO_6^{2\oplus}$ IC-004925

Hexacarbonyliron(2+)
[34248-86-7]

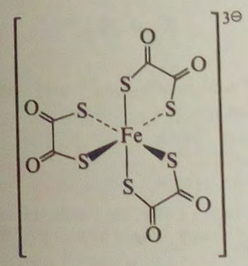
$[Fe(CO)_6]^{2\oplus}$

M 223.9 (ion)
Not well characterised.

Hieber, W. *et al, Angew. Chem.*, 1961, **73**, 580 (*synth, ir*)

$C_6FeO_6S_6^{3\ominus}$ IC-004926

Tris(dithiooxalato)ferrate(*III*)(3−)
Tris[*ethanebis*(*thioato*)(*2*−)-S,S']*ferrate*(*3*−), *9Cl*

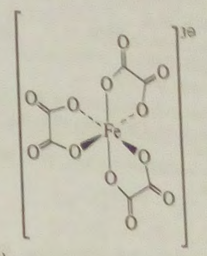


M 416.3 (ion)
Early (1912) ref. formulates $PhNH_3^{\oplus}$ salt incorrectly as Fe(*II*) salt. Violet in soln. Reacts with metal electrophiles to form eg. Tris[bis(triphenylphosphine) silver]tris[μ-(dithiooxalato)]iron(*III*), IC-015933.
Ba,K salt, tetrahydrate: [28628-06-0].
Photosensitive imaging material.
Tris-Ph_4P salt: [94283-06-4].
Violet cryst. + $3MeNO_2$ ($MeNO_2$). Mp 104-107°. μ_{eff} = 2.30μ_B.
Tris[*bis*(*triphenylphosphine*)*copper*(*1*+)] *salt:* see *Tris*[*bis*(*triphenylphosphine*)*copper*]*tris*[μ-(*dithiooxalato*)] *iron*(III), *IC-015936*
Tris[*bis*(*triphenylphosphine*)*silver*(*1*+)] *salt:* see *Tris*[*bis*(*triphenylphosphine*)*silver*]*tris*[μ-(*dithiooxalato*)] *iron*(III), *IC-015933*
[57091-13-1]

Robinson, C.S. *et al, J. Chem. Soc.*, 1912, 62 (*synth*)
Coucouvanis, D. *et al, J. Am. Chem. Soc.*, 1970, **92**, 3004 (*reactivity, electrochem*)
Coucouvanis, D. *et al, J. Am. Chem. Soc.*, 1973, **95**, 5556 (*synth, magnetism, reactivity, ir*)
Birchall, T. *et al, Inorg. Chem.*, 1976, **15**, 376 (*mössbauer*)
Folkesson, B. *et al, J. Electron Spectrosc. Relat. Phenom.*, 1984, **34**, 319 (*esca*)
Japan. Pat., 58 200 234, (1984); *CA*, **100**, 148635q (*use*)

$C_6FeO_{12}^{3\ominus}$ IC-004927

Tris(oxalato)ferrate(*III*)(3−)
Tris[*ethanedioato*(*2*−)-O,O']*ferrate*(*3*−), *9Cl. Ferrioxalate*
[15321-61-6]



M 319.9 (ion)
Octahedral anion. May be resolved. Easily prepared Fe(*III*) complex. Widely used in student experiments. Obt. by H_2O_2 oxidn. of Fe(II) oxalate in presence excess oxalate. Undergoes photoreduction to Fe(*II*). Photocatalyst for a range of reactions. μ_{eff} = 5.95μ_B.
Tri-Na salt: [5936-14-1]. *Ferric sodium oxalate. Sodium ferrioxalate*
Green cryst.
Tri-K salt: [14883-34-2]. *Ferric potassium oxalate. Iron*(II) *potassium oxalate. Potassium ferrioxalate*
$C_6FeK_3O_{12}$ M 437.2
Commercially available for actinometry. Green. Forms a trihydrate.
Tri-NH_4 salt: [14221-47-7]. *Ferric ammonium oxalate. Ammonium ferrioxalate*
Green. Forms a trihydrate.
▷ LJ8932000.
[5936-11-8, 15187-32-3]

Werner, A., *Ber.*, 1912, **45**, 3061 (*resol*)
Weinland, R. *et al, Z. Anorg. Allg. Chem.*, 1921, **117**, 64 (*synth*)
Palmer, W.G., *Experimental Inorganic Chemistry*, C.U.P., 1954 (*synth*)
Herpin, P., *Bull. Soc. Fr. Minéral. Cristallogr.*, 1958, **81**, 245 (*cryst struct*)
Gerloch, M. *et al, J. Chem. Soc. A*, 1969, 1422 (*magnetism*)

$C_6Fe_2I_2O_6$ IC-004928

Hexacarbonyldi-μ-iododiiron, 9Cl
Bis(*tricarbonyliron iodide*)
[36190-47-3]
As Di-μ-bromohexacarbonyldiiron, IC-004862 with X = I

M 533.5
Dark-red needles. Mp 53° dec.

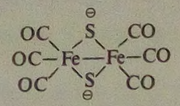
Koerner von Gustorf, E. *et al, Z. Naturforsch., B*, 1972, **27**, 140 (*synth, ir, uv*)

$C_6Fe_2O_6S_2^{2\ominus}$ IC-004929

Hexacarbonyldi-μ-thioxodiferrate(2−), 10CI

Hexacarbonyl[μ-(dithio)]diferrate(2−), 9CI

[69480-73-5]



M 343.8 (ion)

Generated from Hexacarbonyl[μ-(dithio-*S,S′*:*S,S′*)]diiron, IC-004930 with cheavage of S—S bond and used *in situ*.

Di-Li salt: [74438-48-5].
Emerald-green soln. in THF.

Di-K salt: [79255-02-0].
Deep-green soln. in THF.

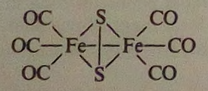
Bayer, E. *et al*, *Eur. J. Biochem.*, 1969, **8**, 4963 (*synth*)
Seyferth, D. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 508; 1981, **103**, 5103 (*synth, use*)
Seyferth, D. *et al*, *J. Organomet. Chem.*, 1980, **192**, C1; 1981, **204**, 333 (*synth, use*)

$C_6Fe_2O_6S_2$ IC-004930

Hexacarbonyl[μ-(dithio-*S,S′*:*S,S′*)]diiron, 9CI

Hexacarbonyldithioxodiiron, 10CI, 9CI. (*μ-Dithio*)*bis(tricarbonyliron)*

[14243-23-3]



M 343.8

Volatile ruby-red prisms. Mp 46.5°. Subl. 40° *in vacuo*. Reduced by Na/THF to Hexacarbonyldi-μ-thioxodiferrate(2−), IC-004929.

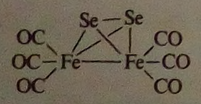
Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **296**, 91 (*synth, ir, uv*)
Wei, C.-H. *et al*, *Inorg. Chem.*, 1965, **4**, 1 (*struct*)
Kettle, S.F.A. *et al*, *Inorg. Chem.*, 1977, **16**, 753 (*raman*)
Chaudhuri, M.K. *et al*, *J. Organomet. Chem.*, 1977, **124**, 37 (*ms*)
Seyferth, D. *et al*, *Organometallics*, 1982, **1**, 125 (*props*)

$C_6Fe_2O_6Se_2$ IC-004931

Hexacarbonyl[μ-(diseleno-*Se,Se′*:*Se,Se′*)]diiron, 10CI

(*μ-Diselenolato*)*bis(tricarbonyliron)*

[76185-26-7]



M 437.6

Air-sensitive deep ruby-red cryst. Mp 39-40.5°.

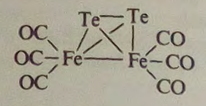
Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **296**, 91 (*synth*)
Campana, C.F. *et al*, *Inorg. Chem.*, 1979, **18**, 3060 (*struct*)
Lesch, D.A. *et al*, *Inorg. Chem.*, 1981, **20**, 3583 (*ir*)
Seyferth, D. *et al*, *J. Organomet. Chem.*, 1981, **204**, 333 (*synth, ms, ir*)

$C_6Fe_2O_6Te_2$ IC-004932

Hexacarbonyl[μ-(ditelluro-*Te,Te′*:*Te,Te′*)]diiron, 10CI

(*μ-Ditellurato*)*bis(tricarbonyliron)*

[76185-27-8]



M 534.9

Labile orange cryst.

Lesch, D.A. *et al*, *J. Organomet. Chem.*, 1980, **199**, C6 (*derivs*)
Lesch, D.A. *et al*, *Inorg. Chem.*, 1981, **20**, 3583 (*synth, ir, ms, nmr*)

$C_6Fe_2O_{12}$ IC-004933

Iron(*III*) oxalate

Ferric oxalate. Iron(III) *ethanedioate. Ferric ethanedioate. Oxalic acid, iron(3+) salt*

[2944-66-3]

$$Fe_2(C_2O_4)_3$$

M 375.7

Fire retardant; used in photographic photosensitive material.

Pentahydrate: [15155-21-2].
$C_6H_{10}Fe_2O_{17}$ M 465.8
Yellow microcryst. powder. V. sol. H_2O; sol. acid; insol. EtOH. Dec. at 100°.

*Gmelin Handbook Inorg. Chem., Syst. No.*59, 1929, **B**, 534 (*rev, bibl*)
Marathe, V.B. *et al*, *Proc. Nucl. Phys. Solid State Phys. Symp., C*, 17th, 1972, 639 (*magnetism, mössbauer*)

$C_6GaO_{12}^{3\ominus}$ IC-004934

Tris(oxalato)gallate(*III*)

Tris[ethanediolato(2−)-O,O′]gallate(3−), 9CI

[52759-65-6]

$$[Ga(C_2O_4)_3]^{3\ominus}$$

M 333.7 (ion)

$[Ga(C_2O_2S_2)_3]^{3\ominus}$ and $[Ga(C_2S_4)_3]^{3\ominus}$ also descr.

Tri-K salt: [29646-69-3].
Colourless cryst. (H_2O).

Tri-NH_4 salt: [58927-23-4].
Colourless cryst. (H_2O).

Neogi, P. *et al*, *J. Indian Chem. Soc.*, 1938, **15**, 83 (*synth*)
Dutt, N.K. *et al*, *Z. Anorg. Allg. Chem.*, 1957, **293**, 195 (*thermodyn*)
Hester, R.H. *et al*, *Inorg. Chem.*, 1964, **3**, 513 (*raman*)
Kul'ba, F.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 365 (*thermodyn data*)
Dutt, N.K. *et al*, *J. Indian Chem. Soc., Sect. A*, 1976, **14**, 491 (*iga*)
Gouteron, J., *J. Inorg. Nucl. Chem.*, 1976, **38**, 55 (*ir, raman*)
Dietzsch, W. *et al*, *Z. Chem.*, 1981, **21**, 269 (*analogues*)

$C_6Ga_2O_{12}$ IC-004935

Gallium(*III*) oxalate

Ethanedioic acid, gallium salt (3:2), 10CI

[70764-38-4]

$$Ga_2(C_2O_4)_3$$

M 403.5

Synth. from hydrate. Colourless hygroscopic solid.

Hydrate: Synth. from $Ga(NO_3)_3$ + $H_2C_2O_4$. Loses H_2O at 170°.

Complex with oxalic acid (1:3), trihydrate:
Hexakis(oxalato)digallate(6−) hexa-H compd., trihydrate
$C_{12}H_{12}Ga_2O_{27}$ M 727.6
Synth. from $Ga(NO_3)_3$ + $H_2C_2O_4$ at pH 0.8-2.5.
Colourless cryst. (H_2O). Formulated as $H_6[Ga_2(C_2O_4)_6]$ $3H_2O$.

Pajakoff, S., *Monatsh. Chem.*, 1969, **100**, 280 (*purifn complexes*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 1106.
Kul'ba, F.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 365 (*thermodyn*)

$C_6Gd_2O_{12}$ IC-004936

Gadolinium(*III*) oxalate

Tris(oxalato)digadolinium(III). *Tris(ethanedioato) digadolinium*(III)

[867-64-1]

$$Gd_2(C_2O_4)_3$$

M 578.5

Decahydrate: [22992-15-0].
$C_6H_{20}Gd_2O_{22}$ M 758.7
Colourless solid. μ_{eff} = 7.84μ_B. Presumed 9-coord.

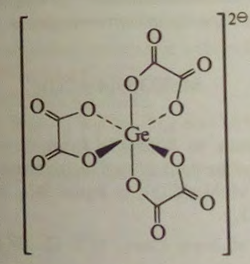
Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth*)
Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Ollendorff, W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Chi, H., *Bull. Chem. Soc. Jpn.*, 1970, **43**, 1703 (*esr*)
Hansson, E., *Acta Chem. Scand.*, 1977, **27**, 823 (*struct*)
Sharov, V.A. *et al*, *Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1979, **5**, 512 (*magnetism*)
Kartha, V.B. *et al*, *Indian J. Phys., B*, 1980, **54**, 36 (*ir, raman*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6GeO_{12}^{2\ominus}$ IC-004937

Tris(oxalato)germanate(*IV*)(2−)

Tris[ethanedioato(2−)-O,O′]germanate(2−), 9CI

[46934-44-5]



M 336.6 (ion)

Di-K salt: [12077-12-2].
Synth. from GeO_2, $K_2C_2O_4.H_2O$ and $2(H_2C_2O_4.2H_2O)$ refluxed in aq. soln. White monoclinic cryst. V. sol. H_2O; insol. EtOH, MeOH, $CHCl_3$, Et_2O. Dec. at 180° with loss of CO_2.

Hexaamminechromium(III) *salt (2:3):* Synth. from $[Cr(NH_3)_6]^{3\oplus}$ soln. and GeO_2 in $H_2C_2O_4$. Yellow rhombic-shaped cryst.

Hexaamminecobalt(III) *salt (2:3):* [17410-70-7].
Synth. from GeO_2 in $H_2C_2O_4$ and $[Co(NH_3)_6]^{3\oplus}$ soln. Orange yellow rhombic-shaped cryst. Sol. H_2O (0.15g per 100 cm^3).

Di-H compd.: [54438-95-8].
Synth. from $H_2C_2O_4.2H_2O$ (aq.) and GeO_2. White silky prisms + $6H_2O$. Dehydrates at 80→170°, dec. to $Ge(C_2O_4)_2$ at 180→210°.

Bis-Et_4N salt: [23301-72-6].
White cryst. V. sol. MeOH. Mp 231-232°.

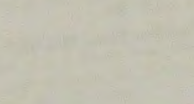
[17374-62-8, 17475-90-0]

Inorg. Synth., 1966, **8**, 35 (*synth, K salt*)
Dean, P.A.W. *et al*, *J. Chem. Soc. A*, 1969, 363 (*synth, ir, raman*)
Breet, E.L.J. *et al*, *Inorg. Chim. Acta*, 1974, **9**, 177, 183; 1980, **40**, 153 (*photol, kinetics*)
Shkodina, T.B. *et al*, *Zh. Neorg. Khim.*, 1974, **19**, 2918; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 1595 (*H compd, synth, ir, struct*)
Kurnevich, G.I. *et al*, *Zh. Prikl. Spektrosk.*, 1974, **21**, 755 (*ir*)
Jorgensen, N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 2051 (*cryst struct, K salt*)
McCrory-Joy, C., *Electrochim. Acta*, 1985, **30**, 51.

$C_6HFe_2NO_6S$ IC-004938

Hexacarbonyl[μ-(η²-thionitrosylhydride-*N,S*)]diiron, 11CI

[88253-20-7]



M 326.8

Complex of Sulphimide HN=S, unknown in free state. Air-stable orange cryst. (pentane). Mp 46-49°. Ir ν_{CO} 2080s, 2040vs, 2000vs, 1995s, 1985m, 1978w cm^{-1} (pentane).

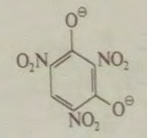
Herberhold, M. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 80 (*synth, ms, ir, pmr*)
Organomet. Synth., 1986, **3**, 273 (*synth, ir, pmr, ms*)

$C_6HN_3O_8Pb$ IC-004939

Lead(*II*) styphnate

2,4,6-Trinitro-1,3-benzenediol, lead(2+) salt(1:1), 9CI. Tricinat

[15245-44-0]



M 450.2

Synth. from styphnic acid + $Pb(NO_3)_2$. Primary explosive used in detonators, blasting caps and percussion primers. Orange-yellow cryst; forms a monohydrate that exists in two polymorphs. Mp 311° dec.

▷ V. sensitive explosive. Shock sensitive. Explodes at 311°.

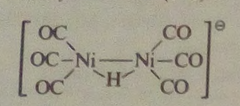
[66778-13-0]

Zingaro, R.A., *J. Am. Chem. Soc.*, 1954, **76**, 816 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley, N.Y., 1978-1984, **19**, 493 (*use*)
Pierce-Butler, M.A., *Acta Crystallogr., Sect. B*, 1982, **38**, 3100 (*cryst struct, hydrate*)
Pierce-butler, M.A., *Acta Crystallogr., Sect. C*, 1984, **40**, 63 (*cryst struct, hydrate*)

$C_6HNi_2O_6^{\ominus}$ IC-004940

Hexacarbonyl-μ-hydrodinickelate(1−)

μ-Hydridohexacarbonyldinickelate(1−)



M 286.4 (ion)

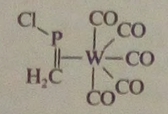
Bis(triphenylphosphine)iminium salt: [71456-74-1].
Cryst. (heptane/THF).

Longoni, G. *et al, J. Organomet. Chem.*, 1979, **174**, C41 (*struct, synth*)
Cerriotti, A. *et al, Inorg. Chem.*, 1983, **22**, 1595 (*synth, ir*)

$C_6H_2ClO_5PW$ IC-004941

Pentacarbonyl(η²-methylenephosphinous chloride) tungsten, 11CI

[100851-76-1]



M 404.3
Deriv. of transient $ClCH_2{=}P$. Highly reactive; gives isolable products with MeOH, 2,3-dimethylbutadiene and 1,4-diphenylbutadiene. Characterised spectroscopically. Ir ν_{CO} 2092m, 1992vs, 1986s, 1970vs, 1944br cm^{-1} (decalin).

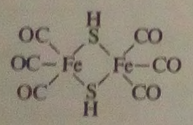
Deschamps, B. *et al, J. Chem. Soc., Chem. Commun.*, 1985, 1010 (*ir, pmr, cmr, P-31 nmr, reactions*)
Deschamps, B. *et al, J. Organomet. Chem.*, 1988, **354**, 83 (*pmr, cmr, P-31 nmr*)

$C_6H_2Fe_2O_6S_2$ IC-004942

Hexacarbonyldi-μ-mercaptodiiron, 10CI

Hexacarbonylbis(μ-hydrothioxo)diiron

[71004-55-2]



M 345.9
V. air-sensitive ruby-red cryst. Mp 62-64° dec., Mp 97-99°. Mixt. of 3 isomers.

Gmelin Handbook Inorg. Chem., 1979, **C1**, 81 (*rev, bibl*)
Seyferth, D. *et al, J. Organomet. Chem.*, 1980, **192**, C1; 1981, **218**, C34 (*synth, pmr, ir, props*)

$C_6H_3BCrNO_5^{\ominus}$ IC-004943

Pentacarbonyl[(cyano-*C*)trihydroborato(1−)-*N*] chromate(1−), 9CI

$[(OC)_5CrNCBH_3]^{\ominus}$

M 231.9 (ion)

Me_4N salt: [52138-78-0].
Yellow cryst. Mp >170° dec.

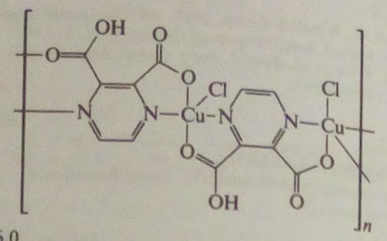
King, R.B. *et al, J. Organomet. Chem.*, 1974, **65**, 71 (*synth, ir, nmr*)

$C_6H_3ClCuN_2O_4$ IC-004944

Chloro[2,3-pyrazinedicarboxylato(1−)]copper(*II*)

Hydrogen chloro[2,3-pyrazinedicarboxylato(2−)-N^1,O^2] cuprate(1−), 9CI

[79329-64-9]



M 266.0
Infinite linear chains with 5-coord. Cu. Green octahedral cryst. (aq. HCl). Exhibits ferromagnetic intrachain exchange.

O'Connor, C.J. *et al, Inorg. Chem.*, 1982, **21**, 64 (*synth, cryst struct, magnetism*)
Burriel, R. *et al, Inorg. Chem.*, 1985, **24**, 3706 (*magnetism*)

$C_6H_3MnNO_4^{\ominus}$ IC-004945

Tetracarbonyl(isocyanomethane)manganate(1−), 9CI

[57195-92-3]

$[(OC)_4MnCNMe]^{\ominus}$

M 208.0 (ion)

Na salt: [75687-67-1].
Synth. from $MnBr(CO)_4(CNMe)$ and Na/Hg in THF at 0°. Generated and used *in situ* as a light-yellow soln. in THF. Ir ν_{CO} 2118m, 1935s, 1863s, 1837vs, 1786s cm^{-1} (THF).

Adams, R.D., *Inorg. Chem.*, 1976, **15**, 174 (*synth, ir*)

$C_6H_3MnO_7S$ IC-004946

Pentacarbonyl(methanesulfinato-*O*)manganese, 9CI

(Methanesulfinato)pentacarbonylmanganese

[37988-76-4]

$MeS(O)OMn(CO)_5$

M 274.0
Rearranges in soln. to *S*-bonded form, Pentacarbonyl(methylsulfonyl)manganese, IC-004947. Synth. from $MeMn(CO)_5$ in liquid SO_2. Not isol. Pmr δ 2.28 ppm (SO_2).

Jacobson, S.E. *et al, Inorg. Chem.*, 1973, **12**, 717 (*synth, ir, pmr*)

$C_6H_3MnO_7S$ IC-004947

Pentacarbonyl(methylsulfonyl)manganese

[19694-44-1]

$MeS(O)_2Mn(CO)_5$

M 274.0
Synth. from $HMn(CO)_5$ and CH_2SO_2 or from $MeMn(CO)_5$ and liquid SO_2. Colourless or pale-yellow cryst. ($CHCl_3$/pentane). Mp 115°. Pmr δ 3.09 ppm (SO_2). Ir ν_{CO} 2139m, 2090w, 2059s, 2044s, 2027m cm^{-1} (CCl_4). Subl. *in vacuo*.

Hartman, F.A. *et al, Inorg. Chem.*, 1968, **7**, 1504 (*synth, ir, pmr*)
Jacobson, S.E. *et al, Inorg. Chem.*, 1973, **12**, 717 (*isom*)
Lorenz, I.-P. *et al, J. Organomet. Chem.*, 1979, **182**, 375 (*synth, ir, pmr, ms*)

$C_6H_4CdN_2O_4$ IC-004948

Bis(cyanoacetato-*N,O*)cadmium

Cadmium cyanoacetate

[52680-39-4]

$(N{\equiv}CCH_2COO)_2Cd$

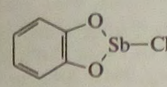
M 280.5
3-D polymer in solid state with approx. octahedral Cd (1 N + 5 O). Hygroscopic colourless plates (H_2O).

[53800-20-7]
Post, M.L. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 285 (*synth, cryst struct*)

$C_6H_4ClO_2Sb$ IC-004949

2-Chloro-1,3,2-benzodioxastibole

[4442-68-6]



M 265.2
Probably polymeric based on -Cl-Sb-Cl-Sb-Cl chain.

Homopolymer: [69860-42-0].
Cryst. (MeCN). Mp >300°.

Anchisi, C. *et al, J. Heterocycl. Chem.*, 1976, **13**, 1033; 1982, **19**, 141 (*synth, reactions, uses*)
Barnard, P.W.C. *et al, Inorg. Chim. Acta*, 1979, **32**, L77 (*ir, raman, cryst struct*)
Maccione, A. *et al, J. Heterocycl. Chem.*, 1983, **20**, 1397 (*uses*)
Podda, G. *et al, J. Heterocycl. Chem.*, 1984, **21**, 1789 (*uses*)
Alonzo, G. *et al, Can. J. Spectrosc.*, 1985, **30**, 21 (*mössbauer*)
McEwen, W.E. *et al, Phosphorus Sulfur*, 1988, **36**, 153 (*pmr, reactions*)

$C_6H_4CrMnN_6O_2^{\ominus}$ IC-004950

Hexakis(μ-cyano)]diaquamanganate(*II*)]chromate(*III*) (1−)

$[Cr(CN)_6Mn(OH_2)_2]^{\ominus}$

M 299.0 (ion)
Anion struct. comprises polymeric network of *trans*-$Mn(OH_2)_2(NC)_4$ and $Cr(CN)_6$.

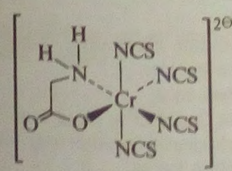
Me_4N salt, 11CI: [102567-08-8].
Synth. from $MnCl_2$, $K_3Cr(CN)_6$ and $[Me_4N]Cl$ in H_2O. Green-yellow plates + $2H_2O$.

Witzel, M. *et al, Z. Naturforsch., B*, 1985, **40**, 1344 (*synth, cryst struct*)

$C_6H_4CrN_5O_2S_4^{2\ominus}$ IC-004951

(Glycinato-*N,O*)tetrakis(thiocyanato-*N*)chromate(*III*) (2−)

Glycinatotetraisothiocyanatochromate(III)(2−)



M 358.3 (ion)
Octahedral anion. Similar spp. known with other amino acids.

Di-K salt: [25591-34-8].

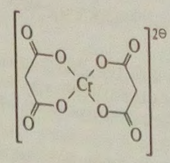
Mp 162°. Ir ν_{CN} 2113, 2089, ν_{CS} 748 cm^{-1}.
Contreras, G. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 127, 1295 (*synth, uv-vis*)

$C_6H_4CrO_8^{2\ominus}$ IC-004952

Bis(propanedioato-*O,O'*)chromate(*II*)(2−)

Bis(malonato)chromate(II)(2−), *8CI*

[28161-98-0]



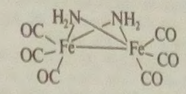
M 256.0 (ion)

Di-Na salt: Blue cryst. + $4H_2O$. μ_{eff} = 4.8μ_B (298K).
Fukuda, Y. *et al, Bull. Chem. Soc. Jpn.*, 1970, **43**, 745 (*stability const*)
Micskei, K. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1335 (*stability const*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 752 (*rev*)

$C_6H_4Fe_2N_2O_6$ IC-004953

Di-μ-amidohexacarbonyldiiron, 9CI, 8CI

[19705-87-4]



M 311.8
Air-sensitive orange-red needles with aromatic smell. Mp 81.5°. Subl. 40° *in vacuo*.

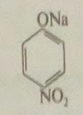
Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1962, **317**, 63 (*synth, ir*)
Dahl, L.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 5422 (*synth, struct, ms*)
Frey, V. *et al, Z. Naturforsch., B*, 1968, **23**, 105 (*synth, struct*)

$C_6H_4NNaO_3$ IC-004954

(4-Nitrophenoxy)sodium

Sodium 4-nitrophenolate, 4-Nitrophenol, sodium salt, 8CI. Sodium p-*nitrophenoxide*

[824-78-2]



M 161.0
Synth. by reaction of 4-nitrophenol with aq. NaOH (or Na_2CO_3) or by hydrolysis of $4\text{-}ClC_6H_4NO_2$ with aq. NaOH. Commercially available (90%). Migrates through organic membranes containing crown ethers. Yellow powder. Sol. H_2O (4.0 g per 100 cm^3 at 25°);insol. $CHCl_3$ (except in presence of crown ethers, cryptands etc.). Mp >300°.

▷ Flammable solid; irritant.

Lopatin, B.V. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1970, 713 (*ir*)
Ueji, S. *et al, Bull. Chem. Soc. Jpn.*, 1977, **50**, 2819 (*uv*)
Marchidan, D.I. *et al, J. Therm. Anal.*, 1978, **14**, 131 (*thermodyn*)
Mishima, M. *et al, Mem. Fac. Sci., Kyushu Univ., Ser. C*, 1980, **12**, 227; *CA*, 1981, **94**, 29971 (*cmr*)

Komiyama, M. *et al*, *Chem. Lett.*, 1984, 1081 (*soly*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3148C (*haz*)

$C_6H_4N_2O_4Zn$ IC-004955

Bis(cyanoacetato-*N,O*)zinc
Zinc cyanoacetate
[71179-00-5]

$Zn(OOCCH_2CN)_2$

M 233.4
Polymeric struct. with octahedral Zn. Catalyst for dimerisation of CH_2=CHCN; cross linking agent for epoxy resins. Colourless cryst. Insol. Me_2CO, MeCN.

[59970-08-0]

Cartwright, M. *et al*, *Inorg. Chim. Acta*, 1979, **34**, 211 (*synth, ir, uv-vis*)

$C_6H_5Br_2OP$ IC-004956

Phenyl phosphorodibromidite, 9CI, 8CI
Phenyl dibromophosphite. Dibromophenoxophosphorus(III)
[70445-77-1]

$PhOPBr_2$

M 283.8
Pungent liq. Bp_{11} 130-132°. n_D^{20} 1.6202.

Frazer, M.J. *et al*, *Chem. Ind. (London)*, 1959, 728 (*synth*)
Fluck, E. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 6363.
Tseng, C.K., *J. Org. Chem.*, 1979, **44**, 2793.
Gloede, J. *et al*, *J. Prakt. Chem.*, 1979, **321**, 1029.
Gloede, J. *et al*, *Z. Anorg. Allg. Chem.*, 1980, **471**, 147 (*P-31 nmr*)
Chauzov, V.A. *et al*, *Zh. Obshch. Khim.*, 1989, **59**, 1294; *J. Gen. Chem. USSR (Engl. Transl.)*, 1989, **59**, 1146 (*P-31 nmr*)

$C_6H_5ClO_2S$ IC-004957

Phenyl chlorosulfite
Chlorosulfurous acid phenyl ester, 9CI
[13165-73-6]

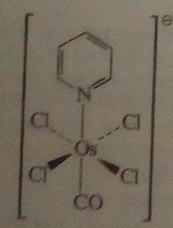
PhOS(O)Cl

M 176.6
Reagent for conversion of aldoximes to nitriles. Bp_{10} 95°.

Bissinger, W.E. *et al*, *J. Am. Chem. Soc.*, 1948, **70**, 2664 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 456 (*use*)

$C_6H_5Cl_4NOOs^{\ominus}$ IC-004958

Carbonyltetrachloro(pyridine)osmate(*III*)(1−)
[80298-13-1]



M 439.1 (ion)
trans-Octahedral anion.
Cs salt: [90709-14-1].
Synth. from $Cs[OsCl_5CO]$ with Py in MeCN in the presence of bentonite and molecular sieve (4Å).
Et_4N salt: [80298-14-2].
Synth. from $[OsCl_4(CO)_2]^{2\ominus}$ or $[OsCl_5CO]^{2\ominus}$ with Py in the presence of bentonite. Ir ν_{CO} 1984vs; ν_{Os-N} 247s; ν_{Os-Cl} 337w, 316vs cm^{-1}.

Greulich, H.G. *et al*, *J. Organomet. Chem.*, 1981, **220**, 201 (*synth, ir, raman, uv*)
Kremer, S., *Inorg. Chim. Acta*, 1984, **85**, 57 (*esr*)

$C_6H_5Cl_4NORu^{\ominus}$ IC-004959

Carbonyltetrachloro(pyridine)ruthenate(*III*)(1−), 9CI
[46136-11-2]

$[RuCl_4(CO)(Py)]^{\ominus}$

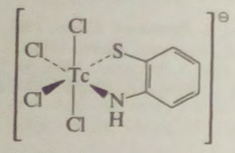
M 349.9 (ion)
Pseudo-octahedral; isomeric form unknown.

Pyridinium salt: Prepd. by treating an aged soln. of ethanolic $RuCl_3.xH_2O$, saturated with CO, with Py. Orange salt. Mp 185°. Ir ν_{CO} 2052, 2046 cm^{-1}; μ_{eff} = 1.8μ_B.
Ph_4As salt: Prepd. by treating a soln. of corresp. pyridinium salt in HCl with $[AsPh_4]Cl$. Orange-brown salt. Mp 175°. Ir ν_{CO} 2042, 2040 cm^{-1}.

Stephenson, T.A. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 945 (*synth, ir, magnetism*)

$C_6H_5Cl_4NSTc^{\ominus}$ IC-004960

[2-Aminobenzenethiolato(2−)-*N,S*] tetrachlorotechnetate(*V*)(1−)

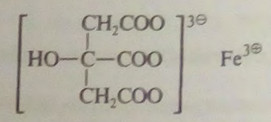


M 363.8 (ion)
Synth. from $TcO(ligand)_2$ + $CHCl_3$.
Tetrabutylammonium salt: [133295-61-1].
Dark blue microcryst (MeOH/HCl). μ_{eff} = 2.86μ_B, hence Tc(*V*).

Cook, J. *et al*, *Inorg. Chem.*, 1991, **30**, 1773 (*synth, cryst struct, ir, magnetism*)

$C_6H_5FeO_7$ IC-004961

Iron(*III*) citrate
Ferric citrate. Iron(III) *2-hydroxy-1,2,3-propanetricarboxylate*
[3522-50-7]



M 244.9
Indefinite composition. Haematinic. Light-sensitive red scales or brown powder.

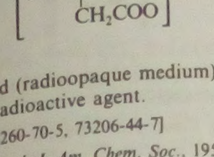
Pentahydrate: [6043-74-9].
Synth. from $Fe_2O_3.nH_2O$ + citric acid. Used for blueprints. Light-sensitive red brown. Insol. EtOH; sol. H_2O. Composition varies.

[28633-45-6]

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1930, **B**, 541 (*bibl*)
Takashima, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1965, **38**, 1688 (*mössbauer*)

$C_6H_5GaO_7$ IC-004962

Gallium citrate
[30403-03-3]



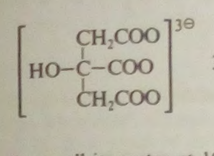
M 258.8
Diagnostic aid (radioopaque medium). ^{67}Ga compd. is used as a radioactive agent.

[41183-64-6, 52260-70-5, 73206-44-7]

Dudley, H.C. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3822; 1951, **73**, 2696 (*synth*)
Brucer, M. *et al*, *Radiology*, 1953, **61**, 534 (*pharmacol*)
Logan, K.J. *et al*, *Int. J. Nucl. Med. Biol.*, 1981, **8**, 271 (*pharmacol*)
Cipriani, C. *et al*, *Inorg. Chim. Acta*, 1984, **92**, 79 (*metab*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 5858.

$C_6H_5Li_3O_7$ IC-004963

Lithium citrate, USAN
2-Hydroxy-1,2,3-propanetricarboxylic acid trilithium salt. Cibalith-S. Demalit. Litarex. Lithonate-S
[6080-58-6]



M 209.9
Tetrahydrate. Loses all its water at 105°. Used in treatment of manic depression.

[919-16-4, 10377-38-5]

Avery, R.C. *et al*, *Proc. Soc. Exp. Biol. Med.*, 1937, **37**, 131 (*activity*)
Glusker, J.P. *et al*, *Acta Crystallogr.*, 1965, **19**, 561 (*cryst struct*)
Loewenstein, A. *et al*, *Spectrochim. Acta*, 1966, **22**, 1939 (*pmr*)
Antonov, L. *et al*, *CA*, 1980, **93**, 142915w (*pharmacol*)

C_6H_5OSb IC-004964

Oxophenylstibine, 10CI
Stibosobenzene
[4519-29-3]

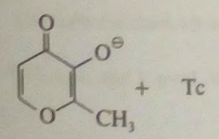
PhSbO

M 214.8
Polymeric. Solid. Insol. Me_2CO.

Blicke, F.F. *et al*, *J. Am. Chem. Soc.*, 1931, **53**, 1025 (*synth*)
Hedges, S.W. *et al*, *J. Chem. Phys.*, 1977, **67**, 4706 (*nqr*)

$[C_6H_5O_3Tc]$ IC-004965

3-Hydroxy-2-methyl-4-pyrone technetium complex
Technetium maltol complex



Minimum formula given. Cationic species not yet characterised. Potential myocardial imaging agent. Pyridinone analogues also reported.

Kanvinde, M.H. *et al*, *J. Nucl. Med.*, 1990, **31**, 908 (*synth, biodistribn*)

$[C_6H_5O_7Tc]$ IC-004966

Technetium citrate
Solcocitran. 2-Hydroxy-1,2,3-propanetricarboxylic acid technetium salt, 11CI

Struct. unknown

Bis-citrate-Tc(*V*) and trinuclear Tc-citrate complexes also know, see Bis(citrato)oxotechnetate(*V*)(3−), IC-007567 and Pentakis(citrato)trioxotritechnetate(*IV*)(9−), IC-012433. Incomplete formula given. Several ill defined complexes produced on reduction of $TcO_4^{\ominus}$/citrate or on reaction of $TcBr_6^{2\ominus}$ with citrate. Imaging kit commercially available. Oxidation state unknown; possibly polymeric.

Gmelin Handbook Inorg. Chem., Syst. No. 69, *Suppl. Vol.*, 1983, **2**, 206 (*rev, bibl*)
Münze, R. *et al*, *Technetium in Chemistry and Nuclear Medicine*, Ed. Deutsch, E. *et al*, Cortina International, Verona, 1983, 51.
Gati, L.J. *et al*, *Nucl. Med. Biol.*, 1986, **13**, 253 (*pharmacol*)

$C_6H_6AlCl_4Cu$ IC-004967

(Benzene)-μ-dichloro(dichloroaluminium)copper(*I*)
[31960-34-6]

$(C_6H_6)Cu[AlCl_4]$

M 310.4
Each Cu is linked to one η^2-C_6H_6 and to three different $[AlCl_4]^{\ominus}$. Colourless v. air- and moisture-sensitive cryst. (C_6H_6).

Turner, R.W. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 1877 (*synth, cryst struct*)
Fichtner, W. *et al*, *Z. Naturforsch., B*, 1980, **35**, 170 (*nqr*)

$C_6H_6BF_3O$ IC-004968

Trifluoro(phenol)boron, 10CI
Trifluoroborane phenol. Phenol compd. with trifluoroborane(1:1), 9CI. Phenol compd. with boron fluoride(BF_3)(1:1), 8CI
[372-44-1]

$PhOH—BF_3$

M 161.9
Catalyst for many types of reactions. Moisture sensitive.

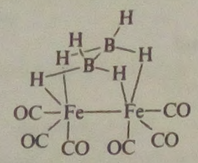
Muetterties, E.L., *J. Am. Chem. Soc.*, 1958, **80**, 4526.
Palko, A.A. *et al*, *J. Chem. Phys.*, 1967, **47**, 2561.
Kobuchi, Y. *et al*, *J. Polym. Sci., Polym. Lett. Ed.*, 1976, **14**, 517.
Ger. Pat., 2 834 126, (1979); *CA*, **90**, 170446u (*use*)
Chmiel-Pela, J., *CA*, 1981, **95**, 189369 (*rev*)

$C_6H_6B_2Fe_2O_6$ IC-004969

Hexacarbonyl[μ-[(1,2-η:1,2-η)-hexahydrodiborato(2−)-H^1:H^1,H^2]]diiron

Hexacarbonyl-μ-(diborane)diiron

[67517-57-1]



M 307.4

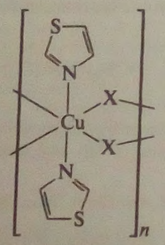
Metallaborane analogous to unknown B_4H_8. Fluxional. Air-sensitive yellow-brown liq. (isol. by low temp. vacuum fractionation). Sol. hexane.

Anderson, E.L. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 4606 (*synth, pmr*)
Fehlner, T.P. *et al*, *Inorg. Chem.*, 1979, **18**, 2325; 1981, **20**, 3291 (*B-11 nmr, pmr, ms, uv-vis, theory*)
Jacobsen, G.B. *et al*, *Inorg. Chem.*, 1987, **26**, 4040 (*synth, pmr, mössbauer, B-11 nmr, ir, ms, theory*)

$C_6H_6Br_2CuN_2S_2$ IC-004970

Dibromobis(thiazole-*N*)copper(*II*), 10CI, 8CI

[29387-44-8]



X = Br

M 393.6

Chain struct. with distorted octahedral Cu and bridging Br. Dark green cryst. (DMF/CH_2Cl_2). Sol. CH_2Cl_2; insol. DMF, EtOH.

Eilbeck, W.J. *et al*, *J. Chem. Soc. A*, 1967, 757 (*synth, uv, ir*)
Hughes, M.N. *et al*, *J. Chem. Soc. A*, 1970, 3015 (*uv, ir*)
Estes, W.E. *et al*, *Inorg. Chem.*, 1978, **17**, 1415 (*cryst struct, synth*)

$C_6H_6Br_3O_7Zr^{\ominus}$ IC-004971

Tris(bromoacetato-*O*)oxozirconate(*IV*)(1−)

$[(BrCH_2COO)_3Zr{=}O]^{\ominus}$

M 521.0 (ion)

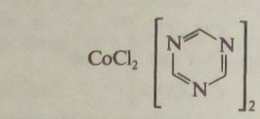
H compd.: [96526-15-7].
$C_6H_7Br_3O_7Zr$ M 522.0
Synth. by heating under reflux $ZrOCl_2$ in excess bromoacetic acid. Solid + $BrCH_2COOH$. Mp > 260°.

Puri, J.K. *et al*, *Inorg. Chim. Acta*, 1985, **97**, 205 (*synth, ir*)

$C_6H_6Cl_2CoN_6$ IC-004972

Dichlorobis(*S*-triazine-N^1)cobalt(*II*), 10CI

[66245-86-1]



M 291.9

Probably octahedral structure with Cl-bridging. Moisture-sensitive pale pink solid.

Johnston, R.D., *Inorg. Chim. Acta*, 1978, **26**, 103 (*synth, uv*)

$C_6H_6Cl_2CuN_2S_2$ IC-004973

Dichlorobis(thiazole)copper(*II*), 10CI, 8CI

[29387-43-7]

As Dibromobis(thiazole-*N*)copper(*II*), IC-004970 with

X = Cl

M 304.7

Chain struct. Turquoise-blue cryst. (DMF/CH_2Cl_2). Sol. CH_2Cl_2; insol. EtOH, Et_2O, C_6H_6, DMF. μ_{eff} = 1.87μ_B.

Eilbeck, W.J. *et al*, *J. Chem. Soc. A*, 1967, 757 (*synth, uv, ir*)
Hughes, M.N. *et al*, *J. Chem. Soc. A*, 1970, 3015 (*uv, ir*)
Estes, W.E. *et al*, *Inorg. Chem.*, 1978, **17**, 1415 (*cryst struct, synth, magnetism*)

$C_6H_6Cl_3O_6Sc$ IC-004974

Scandium chloroacetate

[20753-55-3]

$Sc(OOCCH_2Cl)_3$

M 325.4

Octahedral, polymeric struct. Colourless cryst. Sol. H_2O.

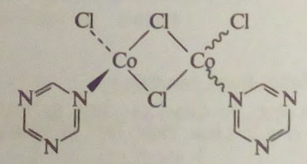
Trihydrate: Colourless cryst. Sol. H_2O.

Pokorny, J. *et al*, *Z. Chem.*, 1972, **12**, 294 (*synth*)
Sugita, Y., *Bull. Chem. Soc. Jpn.*, 1987, **60**, 3441 (*synth, cryst struct*)

$C_6H_6Cl_4Co_2N_6$ IC-004975

Di-μ-chlorodichlorobis(1,3,5-triazine-N^1)dicobalt(*II*), 10CI

[66114-43-0]



M 421.8

Tetrahedral halide bridged dimeric struct. proposed. Moisture-sensitive pale green cryst + $1H_2O$. Paramagnetic.

Monomer: Dichloro(s-*triazine*)*cobalt*(II)
Unknown.

Johnston, R.D. *et al*, *Inorg. Chim. Acta*, 1978, **26**, 103 (*synth, uv, magnetism*)

$C_6H_6Cl_4N_2O_2V$ IC-004976

Tetrachlorobis(2-oxopropanenitrile-*N*)vanadium(*IV*), 11CI

Bis(acetyl cyanide)tetrachlorovanadium(IV)

[104413-79-8]

$VCl_4[N{\equiv}CC(O)CH_3]_2$

M 330.8

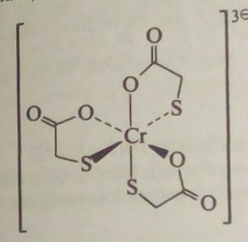
Octahedral. Synth. from VCl_4 and excess CH_3COCN in pet. ether. Dark red solid. Paramagnetic, μ_{eff} = 2.10μ_B (293K). See also μ-Chloroheptachlorotris(2-oxopropanenitrile-*N*)divanadium(*IV*), IC-006474.

Nicholls, D. *et al*, *Inorg. Chim. Acta*, 1986, **115**, L13 (*synth, uv-vis, ir*)

$C_6H_6CrO_6S_3^{3\ominus}$ IC-004977

Tris[mercaptoacetato(2−)]chromate(*III*)(3−), 8CI

Tris(thioglycollato)chromate(III)(3−)



M 322.3 (ion)

Tentative *mer*-struct shown. Cr(*III*) reacts easily with the ligand at temps. above 60°. Complex $(CrL_3)^{3\ominus}$ is formed in pH range 7-10. Blue-green in soln. Not isol.

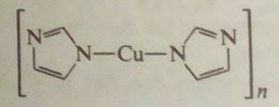
Jacobsen, E. *et al*, *Acta Chem. Scand.*, 1965, **19**, 2379 (*formn, uv-vis*)
Cancellieri, P. *et al*, *Z. Phys. Chem.* (*Frankfurt am Main*), 1968, **62**, 135 (*uv-vis*)

$C_6H_6CuN_4$ IC-004978

Bis(1*H*-imidazolato-N^3)copper(*II*)

Copper(II) *imidazolate*

[29503-37-5]



M 197.6

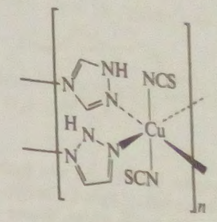
Polymer: the 3-D network of imidazole linked Cu contains Cu in square planar and flattened tetrahedral geometries. Reddish purple solid; blue, green and brown modifications have been reported. Insol. EtOH.

Jarvis, J.A.J. *et al*, *Acta Crystallogr.*, 1960, **13**, 1027 (*cryst struct*)
Bauman, J.E. *et al*, *Inorg. Chem.*, 1964, **3**, 368 (*synth, thermochem*)
Inoue, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1966, **39**, 1352 (*synth, magnetism*)
Weiss, R. *et al*, *Z. Physiol. Chem.*, 1966, **345**, 122 (*synth*)

$C_6H_6CuN_8S_2$ IC-004979

Bis(thiocyanato-*N*)bis-μ-(1*H*-1,2,4-triazole-N^2)copper, 11CI

[99919-16-1]



M 317.8

Two dimensional array with bridging triazole and NCS ligands acting as N donors. Blue-green cryst. (Me_2CO). Sol. Me_2CO, insol. H_2O.

[63654-20-6]

Haasnoot, J.G. *et al*, *Z. Naturforsch., B*, 1977, **32**, 553 (*synth*)
Engelfriet, D.W. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2922 (*cryst struct*)
Inorg. Synth., 1985, **23**, 159 (*synth*)

$C_6H_6F_3NdO_6$ IC-004980

Neodymium(*III*) fluoroacetate

Tris(fluoroacetato)neodymium(III)

[70236-90-7]

$(H_2FCCOO)_3Nd$

M 375.3

Isol. as dimer + $4H_2O$.

Dihydrate (*dimeric*): [62266-57-3].
$C_{12}H_{20}F_6Nd_2O_{16}$ M 822.7
Pink cryst. 9-Coord. dimer, Nd coord. to 2 H_2O, 1 bidentate carboxylate, and 5 bridging carboxylate oxygens; μ_{eff} = 3.63μ_B.

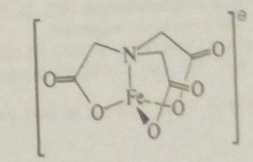
Aslanov, L.A. *et al*, *Koord. Khim.*, 1976, **2**, 1674; *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1976, **2**, 1292 (*cryst struct*)
Singh, M. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 1939 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, D5, 56 (*rev, bibl*)

$C_6H_6FeNO_6^{\ominus}$ IC-004981

Nitrilotriacetatoferrate(*II*)(1−), 8CI

[N,N-*Bis*(*carboxymethyl*)*glycinato*(3−)-N,O,O′,O″]*ferrate*(1−), *11CI*

[31498-52-9]



M 243.9 (ion)

Tetrahedral anion. Reducing agent: H_2S removal from gases. Biologically active, reduces Cytochrome *C*.

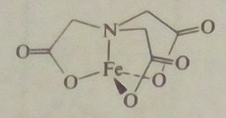
H compd.: [68391-67-3].
Vertes, A. *et al*, *Acta Chim.* (*Budapest*), 1970, **66**, 209; *C.A.*, **74**, 70000b (*mössbauer*)
Wei, J.F. *et al*, *J. Inorg. Biochem.*, 1982, **17**, 237 (*kinetics, use*)

$C_6H_6FeNO_6$ IC-004982

Nitrilotriacetatoiron(*III*), 8CI

[N,N-*Bis*(*carboxymethyl*)*glycinato*(3−)-N,O,O′,O″]*iron*(III), *9CI*

[16448-54-7]



M 243.9

Tetrahedral complex. Usually obt. as a hydrate. Synth. from $FeCl_3$ + Na salt of ligand. Catalyst e.g. for polym. oxidn. Biologically active. Source of Fe. Has applications in desulfurisation, oxidation, fuel cells, photographic bleaches. Sol. H_2O.

▷ Toxic, carcinogenic.

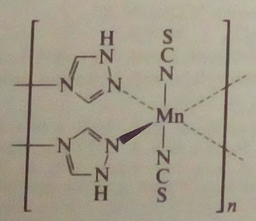
[24323-80-6, 58802-76-9]

Schwarzenbach, G. *et al*, *Helv. Chim. Acta*, 1951, **34**, 1889 (*synth, stability*)
Krishnamurthy, M. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 719 (*synth, ir, magnetism, struct*)
Funahashi, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 479 (*kinetics*)
Rajabalee, F.J.M., *Spectrochim. Acta, Part A*, 1974, **30**, 891 (*ir*)
Stein, G.E. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 2421 (*mössbauer*)
Hamazaki, S. *et al*, *Am. J. Pathol.*, 1986, **123**, 343; *CA*, **105**, 20057p (*tox*)

$C_6H_6MnN_8S_2$ IC-004983

Bis(thiocyanato-*N*)bis(1*H*-1,2,4-triazole-*N*²)manganese(*II*), 11CI

[63654-18-2]



M 309.2

Polymeric chain struct. Synth. by rapid addition of aq. $[NH_4]SCN$ to aq. $Mn(NO_3)_2.6H_2O$ and 1,2,4-triazole. Colourless cryst., single cryst. are pale green. Magnetic props. have been studied in detail.

[99527-45-4]

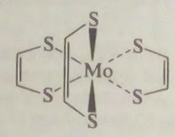
Engelfriet, D.W. *et al*, *Z. Naturforsch., A*, 1977, **32**, 783; 1978, **33**, 848; 1980, **35**, 1387 (*cryst struct, magnetism*)
Haasnoot, J.G. *et al*, *Z. Naturforsch., B*, 1977, **32**, 533 (*synth, ir*)
Mulder, C.A.M. *et al*, *Phys. Lett. A*, 1982, **87**, 303 (*cryst struct, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 63 (*rev, bibl*)

$C_6H_6MoS_6$ IC-004984

Tris[1,2-ethenedithiolato(2−)-*S*,*S*′]molybdenum(*VI*), 11CI, 10CI, 9CI

Molybdenum dithioglyoxal. Tris(*dithioglyoxal*)*molybdenum*(VI)

[24926-09-8]



M 366.4

Trigonal prism. Synth. from Na_2MoO_4 + $Na_2[SCH{=}CHS]$. Semiconductor. Dark, air-stable cryst. (CH_2Cl_2). Sol. CH_2Cl_2, $CHCl_3$. Mp 76° dec. ρ 1.4 x 10^{12} Ω cm.

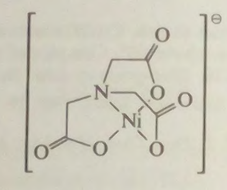
Schrauzer, G.N. *et al*, *Chem. Ind. (London)*, 1965, 1464 (*synth, ir*)
Smith, A.E. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 5798 (*cryst struct*)
Schrauzer, G.N. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 3235 (*synth, ir, uv*)
Rosa, E.J. *et al*, *J. Phys. Chem.*, 1969, **73**, 3132 (*props*)

$C_6H_6NNiO_6^{\ominus}$ IC-004985

Nitrilotriacetatonickelate(*II*)(1−), 8CI

N,N-*Bis*(*carboxymethyl*)*glycinatonickelate*(II)(*1*−), *9CI*. [*Tris*(*2-carboxymethyl*)*amine*]*nickelate*(II)(*1*−)

[16448-53-6]



M 246.8 (ion)

Well known in soln. but little studied in solid state.

Na salt, monohydrate: [54112-02-6].
$C_6H_8NNaNiO_7$ M 287.8

K salt: [63640-18-6].
$C_6H_6KNNiO_6$ M 285.9
Electrolyte component for Au—Ni alloy electrodeposition.

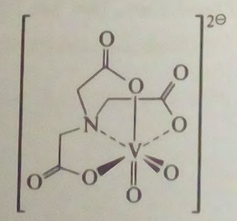
Rajabalee, F.J., *Spectrochim. Acta, Part A*, 1974, **30**, 891 (*synth, ir*)
Bell, C.F., *Principles and Applications of Metal Chelation*, Clarendon, Oxford, 1977.

$C_6H_6NO_8V^{2\ominus}$ IC-004986

(Nitrilotriacetato)dioxovanadate(*V*)(2−)

[N,N-*Bis*(*carboxymethyl*)*glycinato*(3−)-N,O,O′,O″]*dioxovanadate*(V)(2−), *11CI*

[59368-60-4]



M 271.0 (ion)

Octahedral.

Di-K salt: [73636-51-8].

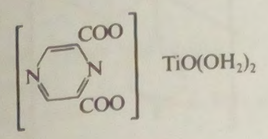
Synth. from Aqua(nitrilotriacetato)oxovanadate(*IV*) (1−), IC-005021 and KNO_2 in H_2O. Yellow hygroscopic solid + $3H_2O$.

Nishizawa, M. *et al*, *Inorg. Chem.*, 1980, **19**, 2284 (*synth*)
Lagrange, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 239 (*kinetics*)

$C_6H_6N_2O_7Ti$ IC-004987

Diaquaoxo[2,6-pyrazinedicarboxylato(2−)-*N*¹,*O*²,*O*⁶]titanium(*IV*), 11CI

[97895-49-3]



M 266.0

Octahedral, detailed arrangement not known. Synth. by adding $TiCl_4$ to a cold aq. soln. of the ligand, then heating to 50°. Colourless solid.

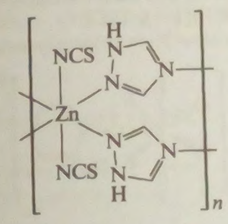
Ventur, D. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **524**, 40 (*synth, ir*)

$C_6H_6N_8S_2Zn$ IC-004988

Bis(thiocyanato-*N*)bis(1*H*-1,2,4-triazole-*N*²)zinc

Bis(1*H*-*1,2,4-triazole*)*zinc dithiocyanate*

[63654-16-0]



M 319.6

2D polymer in solid state with octahedral Zn, 2,4-bridging triazole molecules and NCS-groups acting as N-donors on either side of the plane. H-bonding between layers. White cryst. (H_2O).

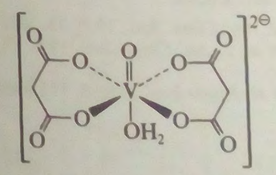
[99527-47-6]

Haasnoot, J.G. *et al*, *Z. Naturforsch., B*, 1977, **32**, 533 (*synth, ir*)
Engelfriet, D.W. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2922 (*cryst struct*)
Inorg. Synth., 1985, **23**, 157 (*synth*)

$C_6H_6O_{10}V^{2\ominus}$ IC-004989

Aquaoxobis[propanedioato(2−)-*O*,*O*′]vanadate(*IV*)(2−), 11CI

Aquabis(*malonato*)*oxovanadate*(IV)(2−). *Oxobis*(*malonato*)*aquovanadate*(IV)



M 289.0 (ion)

Octahedral.

N,N,N′,N′-Tetramethylethylenediammonium salt: [75474-45-2].

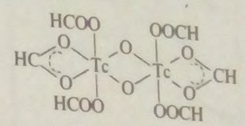
Synth. by dissolving $VO(CO_3)$, malonic acid and $Me_2NCH_2CH_2NMe_2$ (1:1:1) in MeOH. Blue solid.

Tomiyasu, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 2843 (*props*)
Pajunen, A. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 2425 (*synth, cryst struct*)
Collison, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 1705 (*esr*)

$C_6H_6O_{14}Tc_2$ IC-004990

Hexakisformatodi-μ-oxoditechnetium(*V*)

Technetium(V) *formate*



M 499.9

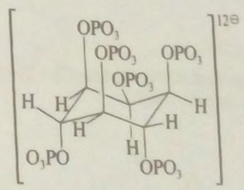
Proposed struct. shown (similar may exist for Tc-acetate, Tc-pivalate). Synth. by electrochem., $BH_4^{\ominus}$ or Sn(*II*) reduction of $TcO_4^{\ominus}$ in formate buffer. Useful precursor for the synthesis of several Tc radiopharmaceuticals. Red complex, exists in soln. in anionic form.

Kennedy, C.M. *et al*, *Appl. Radiat. Isot.*, 1988, **39**, 213, 1159, 1167 (*synth, uv, ir, esr, chromatog, electrochem, rev*)

$[C_6H_6O_{24}P_6Tc^{12\ominus}]$ IC-004991

Phytate technetium complex

Inositol hexaphosphate technetium complex



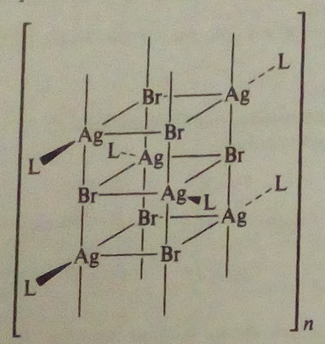
Complex(es) not characterised; product of Sn(*II*) reduction may be a binuclear Tc—Sn—phytate species. Pharmaceutically-useful solns. synth. by Sn(*II*) or electrolytic reduction of $TcO_4^{\ominus}$ in the presence of phytate. Assessed for imaging liver and bones, and for osteosarcoma take-up.

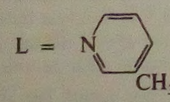
Ikeda, I. *et al*, *J. Nucl. Med.*, 1976, **17**, 389 (*synth*)
Münze, R. *et al*, *Wiss. Fortschr.*, 1980, **30**, 334 (*synth, pharmacol*)
Campbell, J. *et al*, *J. Nucl. Med.*, 1981, **22**, 157 (*interaction with* Sn^{II}, Ca^{II})
Shibata, H. *et al*, *J. Toxicol. Sci.*, 1988, **13**, 151 (*biodistrib*)
Rao, P.N. *et al*, *Eur. J. Nucl. Med.*, 1989, **15**, 162 (*pharmacokinetics*)
Noronha, O.P., *Nucl. Med. Biol.*, 1989, **16**, 261 (*biodistrib*)

C_6H_7AgBrN IC-004992

Bromo(3-methylpyridine-*N*)silver(*I*), 11CI

[95542-93-1]





M 280.9

An infinite array of dimeric $Ag_2Br_2L_2$ units linked face-to-face to forma tube-like struct. Synth. from AgBr + 3-methylpyridine. Cryst.

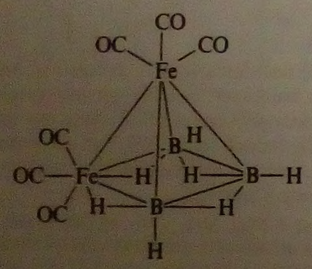
Healey, P.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 111 (*synth, struct*)

$C_6H_7B_3Fe_2O_6$ IC-004993

Hexacarbonyl[μ-[heptahydrotriborato(2 –)]]diiron, 10CI

Diironhexacarbonyltriborane(7)

[71271-99-3]



M 319.2

nido-. Synth. from B_2H_6, $Fe(CO)_5$ and $LiAlH_4$ in dimethoxyethane at 60-70°. Air-sensitive orange cryst. Thermally stable cryst. obt. by annealing polycryst. samples at 45°. V. sol. CH_2Cl_2. Mp 51°.

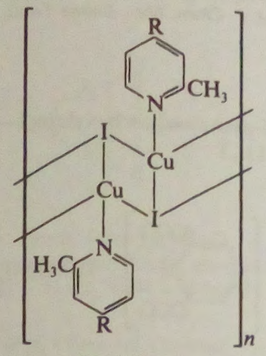
Andersen, E.L. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 4390 (*cryst struct, synth, ir, ms, B-11 nmr, pmr, props*)
Fehlner, T.P. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 4390 (*synth*)
Haller, K.J. *et al*, *Inorg. Chem.*, 1981, **20**, 309 (*cryst struct*)
Andersen, E.L. *et al*, *Inorg. Chem.*, 1981, **20**, 3291 (*pe, uv, theory*)

C_6H_7CuIN IC-004994

Iodo(2-methylpyridine)copper(*I*)

Poly[(2-methylpyridine)iodocopper], *12CI*

[20631-71-4]



R = H

M 283.5

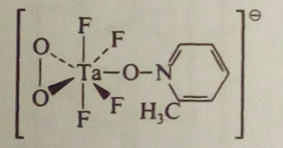
Struct. comprises chains of edge-sharing Cu_2I_2 rhombs with each Cu bound to three I and the N of the Lewis base. Colourless needles.

Rath, N.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 2449 (*synth, cryst struct*)

$C_6H_7F_4NO_3Ta^{\ominus}$ IC-004995

Tetrafluoro(2-methylpyridine-1-oxide-*O*) peroxytantalate(*V*)(1 –), 10CI

Tetrafluoro(α-picoline-N-oxide)peroxytantalate(V)(*1* –)



M 398.0 (ion)

Pentagonal bipyramidal struct.

Et_4N salt: [63871-68-1].
Synth. by dissolving $Et_4N[Ta(O_2)F_4(H_2O)]$ and the ligand in cold MeCN. Colourless, hygroscopic solid (MeCN).

Dewan, J.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 981 (*synth, cryst struct*)

$C_6H_7GaO_8$ IC-004996

Gallium(*III*) hydroxide citrate

$Ga(OH)[OOCCH_2C(OH)(COO)CH_2COOH]$

M 276.8

Used for administration of ^{67}Ga for detection of malignant tumours. White sl. hygroscopic amorphous powder. Sol. H_2O; spar. sol. EtOH.

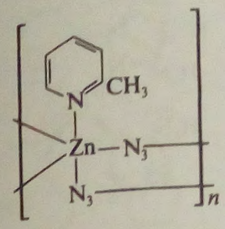
Dudley, H.C., *J. Am. Chem. Soc.*, 1950, **72**, 3822 (*synth*)
Glukson, J.D. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 1679 (*Ga-71 nmr*)
Martell, A.E. *et al*, *Polyhedron*, 1990, **9**, 171 (*thermodyn*)

$C_6H_7N_7Zn$ IC-004997

Diazido(2-methylpyridine)zinc

2-Methylpyridinezinc diazide

[120233-94-5]



M 242.5

Chain struct. with trigonal bipyramidal Zn. Cryst.

▷ Potentially explosive.

Mautner, F.A. *et al*, *Cryst. Res. Technol.*, 1988, **23**, 1477 (*cryst struct*)

$C_6H_7O_4PZn$ IC-004998

Aqua[phenylphosphonato(2 –)-*O,O'*]zinc

Zinc phenylphosphonate monohydrate

[122780-95-4]

$Zn(PhPO_3)(OH_2)$

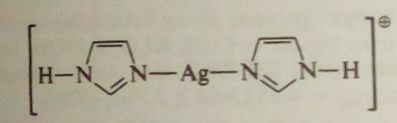
M 239.4

Non-molecular with octahedral zinc in the solid state. Cryst.

Martin, K.J. *et al*, *Inorg. Chim. Acta*, 1989, **155**, 7 (*synth, cryst struct*)

$C_6H_8AgN_4^{\oplus}$ IC-004999

Bis(1*H*-imidazole-N^3)silver(1 +), 10CI



M 244.0 (ion)

Linear cation. Model for metal protein interaction.

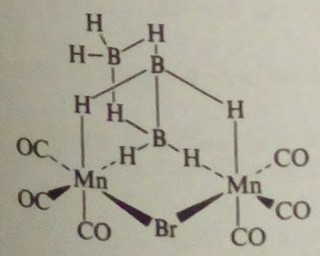
Nitrate: [23757-29-1].
Cryst. Insol. MeOH.

Bauman, J.E. *et al*, *Inorg. Chem.*, 1964, **3**, 368 (*synth, props*)
Antti, C.J. *et al*, *Acta Chem. Scand., Ser. A*, 1971, **25**, 1758 (*cryst struct*)
Acland, C.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 1017 (*cryst struct*)
Symons, M.C.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 709 (*esr*)

$C_6H_8B_3BrMn_2O_6$ IC-005000

μ-Bromohexacarbonyl[μ-[η:η-octahydrotriborato(1 –)]] dimanganese

[74432-08-9]



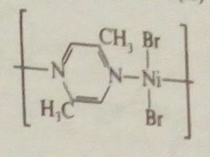
M 398.3

Synth. from $(OC)_3MnB_3H_8$ and $Br_2/AlBr_3$. Mod. air stable red-brown monclinic cryst.

Gaines, D.F. *et al*, *Inorg. Chem.*, 1980, **19**, 2989 (*synth, struct, ms, ir, pmr, B-11 nmr*)

$C_6H_8Br_2N_2Ni$ IC-005001

Dibromo(2,5-dimethylpyrazine)nickel(*II*)



M 326.6

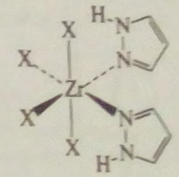
Chain struct. with bridging pyrazines affording *trans*-square planar nickel. Moisture-sensitive intensely purple dichroic cryst. Diamagnetic.

Lever, A.B.P. *et al*, *J. Chem. Soc.*, 1963, 5042; 1964, 4761 (*synth, uv-vis, magnetism*)
Ayres, F.D. *et al*, *Inorg. Chem.*, 1964, **3**, 1303 (*cryst struct*)

$C_6H_8Br_4N_4Zr$ IC-005002

Tetrabromobis(1*H*-pyrazole-N^2)zirconium(*IV*), 11CI

Zirconium tetrabromide bis(pyrazole). Zirconium(IV) *bromide bis(pyrazole)*



cis-form

X = Br

M 546.9

Octahedral.

cis-form [99568-90-8]
Synth. by reacting $TiBr_4$ with excess pyrazole.

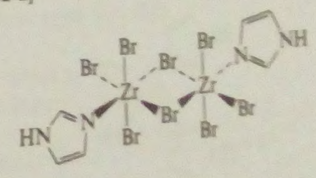
Pazos Perez, M.P. *et al*, *An. Quim., Ser. B*, 1985, **81**, 7 (*synth, ir, raman*)

$C_6H_8Br_8N_4Zr_2$ IC-005003

Di-μ-bromohexabromobis(1*H*-imidazole-N^3) dizirconium(*IV*), 11CI

Tetrabromo(1H-imidazole-N^3*)zirconium*(IV) *dimer. Zirconium*(IV) *bromide imidazole dimer. Zirconium tetrabromide imidazole dimer*

[101307-02-2]



M 957.8

Bi-octahedral. Synth. by mixing solns. of imidazole and $ZrBr_4$. White solid. Insol. MeCN.

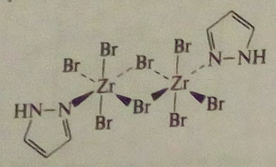
Garcia-Fernandez, M.E. *et al*, *Acta Cient. Compostelana*, 1985, **22**, 197; *CA*, **104**, 160908w (*synth, ir, raman*)

$C_6H_8Br_8N_4Zr_2$ IC-005004

Di-μ-bromohexabromobis(1*H*-pyrazole-N^2)dizirconium(*IV*), 11CI

Tetrabromo(1H-pyrazole-N²)zirconium dimer. Zirconium(IV) bromide pyrazole dimer. Zirconium tetrabromide pyrazole dimer

[99577-65-8]



M 957.8

Synth. by direct reaction of pyrazole with $ZrBr_4$. The monomer *cis*-$ZrBr_4L_2$ may also be synth.

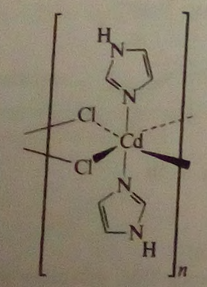
Pazos-Perez, M.P. *et al, An. Quim., Ser. B*, 1985, **81**, 7; *CA*, **104**, 13994t (*synth, ir, raman*)

$C_6H_8CdCl_2N_4$ IC-005005

Dichlorobis(1*H*-imidazole-N^3)cadmium(*II*)

Bis(1H-imidazole-N³)cadmium dichloride. Cadmium(II) chloride bis(imidazole)

[41733-40-8]



M 319.4

Polymeric with approx. octahedral Cd. Colourless cryst. (H_2O).

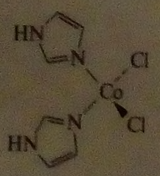
Flook, R.J. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 903 (*synth, cryst struct*)

Ashby, C.I.H. *et al, J. Am. Chem. Soc.*, 1978, **100**, 6057 (*N-14 nqr*)

$C_6H_8Cl_2CoN_4$ IC-005006

Dichlorobis(1*H*-imidazole-N^3)cobalt(*II*), 9CI

[12317-30-5]



M 265.9

Tetrahedral. Blue cryst.

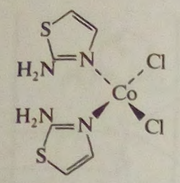
Antti, C.J. *et al, Acta Chem. Scand., Ser. A*, 1972, **26**, 3995 (*synth, cryst struct*)

$C_6H_8Cl_2CoN_4S_2$ IC-005007

Bis(2-aminothiazole)dichlorocobalt(*II*)

Dichlorobis(2-thiazolamine-N³)cobalt(II), 9CI

[38840-69-6]



M 330.1

Tetrahedral around Co. Blue cryst. Paramagnetic.

Duff, E.J. *et al, Inorg. Chim. Acta*, 1972, **6**, 408 (*synth, uv, magnetism*)

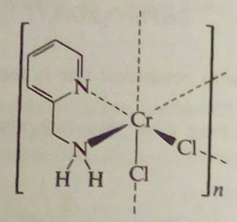
Raper, E.S. *et al, Acta Crystallogr., Sect. B*, 1981, **37**, 928 (*cryst struct*)

$C_6H_8Cl_2CrN_2$ IC-005008

[2-(Aminomethyl)pyridine]dichlorochromium(*II*), 8CI

Dichloro(2-picolylamine)chromium(II)

[27435-75-2]



M 231.0

Chloride-bridged polymer giving octahedral coordination. Synth. from ligand + $CrCl_3.4H_2O$ in EtOH. Light green air-sensitive solid. Sol. DMF dec. Antiferromagnetic complex: μ_{eff} = 4.45 (300K); 3.70μ_B (90K).

Earnshaw, A. *et al, J. Chem. Soc. A*, 1970, 1840 (*synth, magnetism, uv*)

$C_6H_8Cl_2CrN_4$ IC-005009

Dichlorobis(1*H*-pyrazole-N^2)chromium(*II*), 9CI

[58465-92-2]

$CrCl_2(C_3H_4N_2)_2$

M 259.0

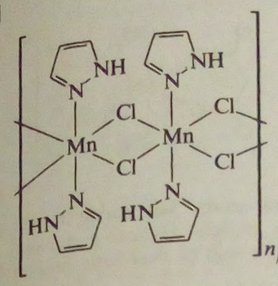
Chloride-bridged polymer with distorted octahedral coordination. Synth. from excess $CrCl_2$ + ligand in EtOH. Air sensitive solid. Sol. DMF; insol. other common org. solvs. μ_{eff} = 4.62 (298K); 4.06μ_B (84K).

Mani, F. *et al, Inorg. Chim. Acta*, 1976, **16**, 163 (*synth, props*)

$C_6H_8Cl_2MnN_4$ IC-005010

Dichlorobis(1*H*-pyrazole-N^2)manganese(*II*), 9CI

[39297-36-4]



M 261.9

Polymeric chain struct. with octahedral Mn. Synth. from hydrated $MnCl_2$ and pyrazole in EtOH. Air-stable, pale pink cryst. Mp > 300°. Paramagnetic, T_N < 1.3K. Magnetic behaviour similar to $MnCl_2py_2$. ΔH_f −63.6kJ mol^{-1}.

Gorder, S. *et al, Acta Crystallogr., Sect. B*, 1970, **30**, 1867 (*cryst struct*)

Witteveen, H.T. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 1535 (*synth, magnetism, esr*)

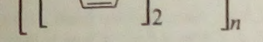
Barvinok, M.S. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 1173 (*props, ir*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 274 (*rev, bibl*)

$C_6H_8Cl_2N_4Ni$ IC-005011

Dichlorobis(1*H*-imidazole-N^3)nickel(*II*), 9CI

[54192-72-2]



M 265.7

***trans*-form** [28678-63-9]

Polymeric. Yellow-green solid. Mp > 300°. Paramagnetic.

[54192-76-6]

Taylor, C.E. *et al, J. Chem. Soc. A*, 1969, 368 (*synth, ir*)

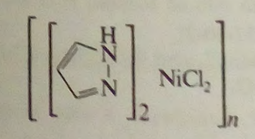
Jansen, J.C. *et al, Z. Naturforsch., B*, 1974, **29**, 527 (*synth, ir*)

Van Dam, J.C. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 713 (*thermochem*)

$C_6H_8Cl_2N_4Ni$ IC-005012

Dichlorobis(1*H*-pyrazole-N^2)nickel(*II*), 9CI

[32592-87-3]



M 265.7

Exists as polymer. Yellow-green cryst. Insol. org. solvs.

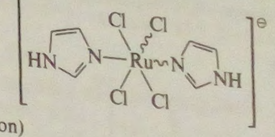
[52242-47-4]

Nicholls, D. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 3871 (*synth*)

Witteveen, H.T. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 913 (*synth, magnetism*)

$C_6H_8Cl_4N_4Ru^{\ominus}$ IC-005013

Tetrachlorobis(1*H*-imidazole-N^3)ruthenate(*III*)(1−), 9CI



M 379.0 (ion)

Config. at Ru not reported. Prepd. by treating $RuCl_3.xH_2O$ in HCl with imidazole.

Imidazolium salt: Orange-yellow cryst.

Králík, F. *et al, Collect. Czech. Chem. Commun.*, 1961, **26**, 1298.

$C_6H_8Cl_4N_4Zr$ IC-005014

Tetrachlorobis(1*H*-pyrazole-N^2)zirconium(*IV*), 11CI

Zirconium(IV) chloride bis(pyrazole)

As Tetrabromobis(1*H*-pyrazole-N^2)zirconium(*IV*), IC-005002 with

X = Cl

M 369.1

Octahedral.

***cis*-form** [99568-89-5]

Synth. from $TiCl_4$ and excess pyrazole.

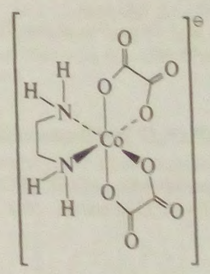
Pazos Perez, M.P. *et al, An. Quim., Ser. B*, 1985, **81**, 7 (*synth, ir, raman*)

$C_6H_8CoN_2O_8^{\ominus}$ IC-005015

Ethylenediaminebis(oxalato)cobaltate(*III*)(1−)

(1,2-Ethanediamine-N,N')bis[ethanedioato(2−)-O,O']cobaltate(III)(1−), 9CI

[23603-95-4]



M 295.0 (ion)

(+)-*form* [20673-37-4]

Na salt: [33516-79-9].

Red-violet cryst. Sol. H_2O.

(−)-*form*

Na salt: [33516-80-2].

Red-violet cryst. Sol. H_2O.

Dwyer, F.P. *et al, J. Am. Chem. Soc.*, 1961, **83**, 1285 (*synth*)

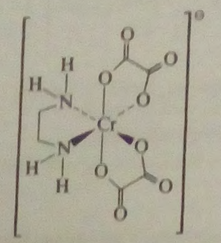
Inorg. Synth., 1972, **13**, 195 (*synth, resol, props*)

$C_6H_8CrN_2O_8^{\ominus}$ IC-005016

(Ethylenediamine)bis(oxalato)chromate(*III*)(1−), 8CI

(1,2-Ethanediamine-N,N′)bis[ethanedioato(2−)-O,O′]chromate(III)(*1*−), *11CI, 10CI,9CI*

[46752-51-6]



Δ-form

M 288.1 (ion)

Isomers racemise at mod. rates in aq. soln.

Δ-form

(+)-form

K salt: [23594-45-8].
Solid + $2H_2O$.

(±)-form

K salt: [15453-41-5].
Cryst. + KI + $2H_2O$ (aq. KI). Double salt.

Bis(ethylenediamine)oxalatochromium(III)(*1*+) *salt:* [14856-29-2].
Can be obt. on irradiation of $[Cr(en)_3]_2(C_2O_4)_3.3H_2O$.
Red cryst. + $2H_2O$. Spar. sol.

[14493-60-8, 21827-84-9, 29985-46-4, 51982-77-5]

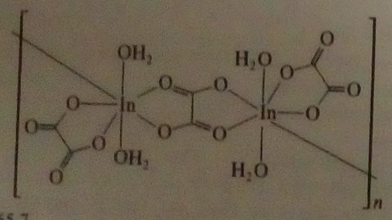
Kaizaki, S. *et al, Bull. Chem. Soc. Jpn.*, 1969, **42**, 988; 1970, **43**, 1100 (*cd, abs config*)
Lethbridge, J.W. *et al, J. Chem. Soc. A*, 1970, 1862 (*cryst struct*)
Andriessen, W.T.M., *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1973, **92**, 1389 (*esr*)
Glasser, L.S.D. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 2065 (*cryst struct, double salt*)

$C_6H_8In_2O_{16}$ IC-005017

μ-(Oxalato-O^1,O^2:O^1,O^2)bis[diaqua(oxalato-$O^1;O^2$)indium]

Tetraaqua[μ-[ethanedioato(2−)-O,O‴:O,O‴]]bis[ethanedioato(2−)-O,O′]diindium, 11CI

[84948-84-5]



M 565.7

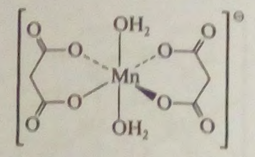
Approx. pentagonal bipyramidal at In with fifth equatorial position occupied by carbonyl O from a neighbouring dimer forming chain struct. White needles + $2H_2O$ (H_2O).

Bulc, N. *et al, Acta Crystallogr., Sect. C*, 1983, **39**, 174 (*synth, cryst struct*)

$C_6H_8MnO_{10}^{\ominus}$ IC-005018

Diaquabis[propanedioato(2−)-*O,O′*]manganate(*III*)(1−)

Diaquabis(malonato)manganate(III)(*1*−)



M 295.0 (ion)

trans-Octahedral anion. Salts stable toward air in solid state; dec by uv light. Hydrol. in aq. soln. to Mn(*III*) unless malonic acid or malonates present. Dec. on heating.

K salt: Now known to be K salt of Methanolbis[propanedioato(2−)-*O,O′*]manganate(*III*)(1−), IC-005721.

K salt, dihydrate: [63313-02-0].
Synth. by addition of a soln. of malonic acid, neutralised with K_2CO_3 to a soln. of Mn(*III*) synth. from $MnSO_4$ and $KMnO_4$. Green cryst.; dimorphic. High spin Mn(*III*) d^4 complex; μ_{eff} = 4.91μ_B (300K).

Cs salt: Obt. by metathesis of corresp. H compd. with Cs_2SO_4. Green solid. μ_{eff} = 5.03μ_B (300K), 5.04μ_B (90K). Various other salts also known.

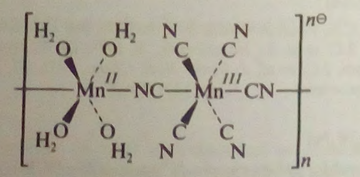
H compd., tetrahydrate: Synth. from $KMnO_4$ in aq. EtOH and malonic acid. Green solid.

[38459-40-4, 63313-02-0]

Cartledge, G.H. *et al, J. Am. Chem. Soc.*, 1940, **62**, 3057 (*synth*)
Bullock, J.I. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 415 (*synth, ir, uv, magnetism*)
d'Ascenzo, G. *et al, Gazz. Chim. Ital.*, 1972, **102**, 132 (*uv*)
Lis, T. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 1943 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 128 (*rev, bibl*)
Lis, T. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 996 (*cryst struct*)
Lis, T. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1980, **54**, 163 (*cryst struct*)

$C_6H_8Mn_2N_6O_4^{\ominus}$ IC-005019

Tetraaquabis(μ-cyano)tetrakis(cyano)dimanganate(1−)



M 338.0 (ion)

Chain anion with almost eclipsed H_2O and CN groups.

Me_4N salt: [86257-80-9].
Synth. from $MnCl_2$ and $[Me_4N]_3Mn(CN)_6$ in H_2O.
Cryst. + $4H_2O$.

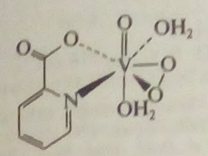
Henkel, H. *et al, Z. Naturforsch., B*, 1984, **39**, 880 (*synth, cryst struct*)

$C_6H_8NO_7V$ IC-005020

Diaquaoxoperoxy(2-pyridinecarboxylato-N^1,O^2)vanadium(*V*), 11CI

Diaquaoxoperoxy(2-picolinato)vanadium(V)

[85082-23-1]



M 257.0

Pentagonal bipyramidal. Synth. from V_2O_5 in 30% H_2O_2 in the presence of picolinic acid at 0°. Reagent/catalyst for non-stereospecific epoxidation of olefins and hydroxylation of aromatic and aliphatic hydrocarbons. Brick-red cryst. Sol. H_2O, common org. solvs.

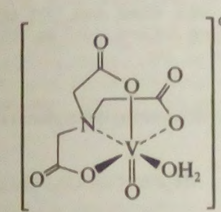
Mimoun, H. *et al, J. Am. Chem. Soc.*, 1983, **105**, 3101 (*synth, cryst struct, ir, reactions*)
Eur. Pat., 97 551, (1984); *CA*, **100**, 174641h (*use*)

$C_6H_8NO_8V^{\ominus}$ IC-005021

Aqua(nitrilotriacetato)oxovanadate(*IV*)(1−)

Aqua[N,N-bis(carboxymethyl)glycinato(3−)-N,O,O′,O″]oxovanadate(IV)(*1*−), *11CI*

[12347-63-6]



M 273.0 (ion)

Na salt: [73711-58-7].
Synth. from the corresp. Ba salt and aq. Na_2SO_4. Blue solid.

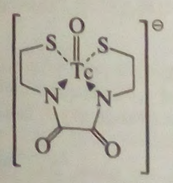
K salt: [72268-05-4].
Synth. by ion exchange from the Ba salt.

Ba salt (2:1): [73711-57-6].
Synth. from $VOSO_4$ and an aq. soln. of the Ba salt of the ligand. Light blue solid + $4H_2O$ (aq. EtOH).

Nishizawa, M. *et al, J. Chem. Soc., Chem. Commun.*, 1979, 707 (*synth, esr*)
Nishizawa, M. *et al, Inorg. Chem.*, 1980, **19**, 2284 (*synth, kinetics*)
Johnson, M.D. *et al, Inorg. Chem.*, 1983, **22**, 1068 (*kinetics*)
Hallmeier, K.H. *et al, Spectrochim. Acta, Part A*, 1986, **42**, 841 (*xanes*)

$C_6H_8N_2O_3S_2Tc^{\ominus}$ IC-005022

[*N,N′*-Bis(2-mercaptoethyl)oxamido(4−)]oxotechnetate(*V*)(1−)



M 319.1 (ion)

Synth. by $S_2O_4^{2\ominus}$ redn. of $TcO_4^{\ominus}$ in EtOH in presence of ligand, or by ligand exchange reaction from $[TcO(OCH_2CH_2O)_2]^{\ominus}$.

Ph_4As salt: [91443-63-9].
Orange cryst. (cyclohexane/CH_2Cl_2). Mp 227-228°.

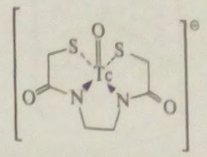
Brenner, D. *et al, Inorg. Chem.*, 1984, **23**, 3793 (*synth, uv, ir, pmr, cmr, ms, electrochem*)

$C_6H_8N_2O_3S_2Tc^{\ominus}$ IC-005023

[*N,N′*-Ethylenebis(2-mercaptoacetamido)(4−)]oxotechnetate(*V*)(1−)

DADS-Tc. Tc-DADS

[75949-44-9]



M 319.1 (ion)

Isomeric with [*N*-(2-Mercaptoacetyl)-*N′*-(2-mercaptoethyl)glycinamido(4−)]oxotechnetate(*V*)(1−), IC-005024 and [*N,N′*-Bis(2-mercaptoethyl)oxamido(4−)]oxotechnetate(*V*)(1−), IC-005022; square pyramidal with Tc 77 pm above the N_2S_2 plane. Parent of series of O=TcN_2S_2 imaging agents. Synth. from $TcO_4^{\ominus}$ by $S_2O_4^{2\ominus}$ reduction in presence of ligand. Diamagnetic.

Tetrabutylammonium salt: [75949-46-1].
Yellow-gold solid.

$MePh_3As$ salt: Yellow solid (Me_2CO aq.).

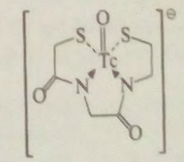
Ph_4As salt: [75949-45-0].
Yellow solid (Me_2CO aq.). Mp 219-222° dec.

[114095-55-5]

Davison, A. *et al, Inorg. Chem.*, 1981, **20**, 1629 (*synth, uv, pmr, ir*)
Jones, A.G. *et al, J. Nucl. Med.*, 1982, **23**, 801 (*pharmacol, ms, cryst struct, hplc*)
Brenner, D. *et al, Inorg. Chem.*, 1984, **23**, 3793 (*synth, electrochem*)
Kasina, S. *et al, J. Med. Chem.*, 1986, **29**, 1933 (*hplc, analogues*)
Bryson, N. *et al, Inorg. Chem.*, 1988, **27**, 2154 (*analogues*)
Dilworth, J.R. *et al, Transition Met. Chem.*, 1990, **15**, 411 (*rev, formn mechanism*)

$C_6H_8N_2O_3S_2Tc^{\ominus}$ IC-005024

[*N*-(2-Mercaptoacetyl)-*N′*-(2-mercaptoethyl)glycinamido(4−)]oxotechnetate(*V*)(1−), 11CI



M 319.1 (ion)

Member of series of diamidodithiolato complexes contg. $TcO^{3\oplus}$ core. Synth. by $S_2O_4^{2\ominus}$ redn. of $TcO_4^{\ominus}$ in presence of ligand, or by ligand exchange reaction of $[TcO(OCH_2CH_2O)_2]^{\ominus}$. Potential renal diagnostic agent.

Ph_4As salt: [91443-61-7].
Yellow cryst. (Me_2CO aq.). Insol. H_2O. Mp 232-235°.

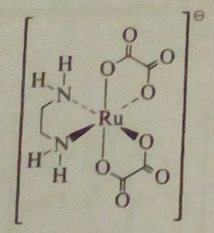
Brenner, D. *et al, Inorg. Chem.*, 1984, **23**, 3793 (*synth, uv, pmr, cmr, ms, electrochem*)

$C_6H_8N_2O_8Ru^{\ominus}$ IC-005025

(Ethylenediamine)bis(oxalato)ruthenate(*III*)(1−)

(1,2-Ethanediamine-N,N′)bis[ethanedioato(2−)-O,O′] ruthenate(III)(*1−*), *9CI. (1,2-Diaminoethane)bis(oxalato) ruthenate*(III)

[46752-56-1]



M 337.2 (ion)

Prepd. by treating Tris(oxalato)ruthenate(*III*)(3−), IC-005659 in H_2O with $[H_3NCH_2CH_2NH_3][C_2O_4]$. Sol. H_2O.

Na salt: Green cryst. + $3H_2O$.

Bis(1,2-ethylenediamine)oxalatoruthenium(1+) salt: see *Bis(ethylenediamine)oxalatoruthenium*(III)(*1+*), *IC-005281*

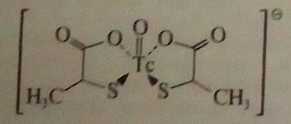
[46752-55-0]

Broomhead, J.A. *et al, J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, magnetism*)
Witschy, J.K. *et al, Inorg. Nucl. Chem. Lett.*, 1969, **5**, 969 (*synth*)

$C_6H_8O_5S_2Tc^{\ominus}$ IC-005026

Bis[2-mercaptopropanoato(2−)-*O,S*]oxotechnetate(*V*) (1−), 10CI

Bis(2-thiolactato)oxotechnetate(V)(*1−*)



M 323.1 (ion)

Square pyramidal anion. Synth. from $TcO_4^{\ominus}$ and 2-mercaptopropanoic acid in HOAc. Potential imaging agent. 2-Mercaptohexadecanoate analogue synth. as a lipophilic alternative.

Ph_4As salt: [78319-73-0].

Brown solid. No well-defined Mp.

Livni, E. *et al, J. Nucl. Med.*, 1981, **22**, 535 (*synth, uv, ir, ms, pmr, props*)

$C_6H_9AlO_6$ IC-005027

Aluminium acetate

Aluminium ethanoate. Acetic acid, aluminium salt (3:1)

[139-12-8]

$Al(OAc)_3$

M 204.1

Synth. from $AlCl_3$ and glacial HOAc or from Al, HOAc + $(CH_3CO)_2O$. Antiseptic, mordant. V. hygroscopic white solid (HOAc). Sol. H_2O; spar. sol. Me_2CO. Range of similar tricarboxylates descr.

Hood, G.C. *et al, J. Am. Chem. Soc.*, 1950, **72**, 2094.
Mehrotra, R.C. *et al, J. Inorg. Nucl. Chem.*, 1956, **2**, 60.
Pande, K.C. *et al, Z. Anorg. Allg. Chem.*, 1956, **286**, 2989 (*synth, related compds*)
Mehrotra, R.C. *et al, Metal Carboxylates*, Academic Press, London, 1983.

$C_6H_9AmO_8^{\ominus}$ IC-005028

Tris(acetato-*O,O′*)dioxoamericate(*VI*)(1−)

$[AmO_2(OAc)_3]^{\ominus}$

M 450.1 (ion)

8-Coord.

Na salt: [41618-84-2].

Cryst. Sol. H_2O. Ir $\nu_{Am=O}$ 914 cm^{-1}.

K salt: Cryst. Sol. H_2O. Isostructural with U analogue.

Zachariasen, W.H., *Acta Crystallogr.*, 1959, **12**, 526 (*cryst struct*)
Grenthe, I., *Acta Chem. Scand.*, 1962, **16**, 1695 (*stability const*)
Vdorenko, V.M. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1973, **209**, 352 (*ir*)
Vdorenko, V.M. *et al, Radiokhimiya*, 1974, **16**, 716; *CA*, **82**, 105013 (*ir*)
Vodoratov, V.A. *et al, Radiokhimiya*, 1985, **27**, 831; *CA*, **104**, 160916 (*use*)

$C_6H_9AsO_3S_6$ IC-005029

Tris(*O*-methyl carbonodithioato-*S,S′*)arsenic

Tris(O-*methyl dithiocarbonato*)*arsenic. Tris*(O-*methyl xanthato*)*arsenic. Arsenic tri*(*methyl xanthate*)

[40934-92-7]

$As[SC(S)OMe]_3$

M 396.4

Cryst. (CH_2Cl_2). Mp 80-81°. Dimorphous.

Khwaja, M.A. *et al, Anal. Chim. Acta*, 1973, **64**, 9 (*synth, props*)
Snow, M.R. *et al, Aust. J. Chem.*, 1987, **40**, 743 (*cryst struct*)

$C_6H_9AuFeNO_4P$ IC-005030

Tricarbonylnitrosyl](trimethylphosphine)aurio]iron, 8CI

[33989-32-1]

$Me_3PAuFe(CO)_3NO$

M 442.9

Mp 86-88° dec.

Casey, M. *et al, J. Chem. Soc. A*, 1971, 2989 (*synth, ir*)

$C_6H_9AuFeNO_7P$ IC-005031

Tricarbonylnitrosyl](trimethyl phosphite-*P*)aurio]iron

[34088-91-0]

$(MeO)_3PAuFe(CO)_3NO$

M 490.9

Mp 50-51° dec.

Casey, M. *et al, J. Chem. Soc. A*, 1971, 2989 (*synth, ir*)

$C_6H_9B_3EuF_{12}N_3$ IC-005032

Tris(acetonitrile)tris(tetrafluoroborato)europium

Tris(methyl cyanide)europium tris(tetrafluoroborate)

[102233-99-8]

$(H_3CCN)_3Eu(BF_4)_3$

M 535.5

In MeCN initiates polym. and oligomerisation of styrene, methylstyrene and 1,3-cyclohexadiene. Air-stable but moisture-sensitive orange cryst. Sol. MeCN. Ir ν_{NC} 2310, 2280 cm^{-1}.

Thomas, R.R. *et al, J. Am. Chem. Soc.*, 1986, **108**, 4096 (*synth, ir, nmr*)

$C_6H_9BiO_3S_6$ IC-005033

Tris(*O*-methyl carbonodithioato-*S,S′*)bismuth, 11CI, 9CI

Tris(*O-methyl dithiocarbonato*)*bismuth. Tris*(O-*methyl xanthato*)*bismuth. Bismuth tri*(*methyl xanthate*)

[41322-43-4]

$Bi[SC(S)OMe]_3$

M 530.5

Cryst. (CH_2Cl_2). Mp 130-131°. Loosely held dimeric struct.

Khwaja, M.A. *et al, Anal. Chim. Acta*, 1973, **64**, 9 (*synth, props*)
Snow, M.R. *et al, Aust. J. Chem.*, 1987, **40**, 743 (*cryst struct*)

$C_6H_9BiO_6$ IC-005034

Bismuth(*III*) acetate

Bismuth triacetate. Acetic acid, bismuth(3+) salt

[22306-37-2]

$Bi(OAc)_3$

M 386.1

Synth. from Bi_2O_3 + AcOH/Ac_2O; or from $BiBr_3$ + TlOAc. Acetylating agent for amines and alcohols. High sensitivity photoimaging compd. Colourless glistening elongated tablets. Insol. H_2O. Mp >250°. Hydrol. by H_2O. Stable at 75° under N_2. Dec. in air on heating.

Rigby, W., *J. Chem. Soc.*, 1951, 793 (*synth*)
Manabe, K. *et al, CA*, 1969, **70**, 61589 (*props*)
Gattow, G. *et al, Z. Anorg. Allg. Chem.*, 1971, **382**, 49 (*synth, ir, uv, pmr, ms, cryst struct*)
Reese, A.L. *et al, J. Org. Chem.*, 1973, **38**, 764 (*use, synth*)
Koch, T.R. *et al, J. Org. Chem.*, 1979, **44**, 157 (*reactions, use*)
Anishchenko, N.I. *et al, Zh. Obshch. Khim.*, 1979, **49**, 1185; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **49**, 1039 (*synth*)

$C_6H_9CeO_6$ IC-005035

Cerium(*III*) acetate

Cerium triacetate. Cerous acetate

[19955-75-0]

$Ce(OAc)_3$

M 317.2

White solid. Sol. C_6H_6, H_2O. Dec. at 308°.

Monohydrate: Air-stable colourless cryst. Sol. H_2O, MeOH. 9-Coordinate Ce, either capped sq. antiprism or tricapped trigonal prism Dec. at 200-300°.

1.5 Hydrate: [79464-05-4].

Colourless cryst. Sol. H_2O. Loses H_2O at 115°.

DMF complex:

$C_9H_{16}CeNO_7$ M 390.3

Colourless cryst. Mp 148-155°. Loses DMF *in vacuo* at 210°.

Tris-urea complex: [41579-90-2].

$C_9H_{21}CeN_6O_9$ M 497.4

Colourless cryst. + $1.5H_2O$. Mp 138°.

Thiourea complex:

$C_7H_{13}CeO_6S_3$ M 429.4

Colourless cryst. + $2H_2O$. Mp 225-226°.

Phen complex:

$C_{18}H_{17}CeN_2O_6$ M 497.4

Yellow cryst. Dec. at 270-272°.

[537-00-8, 72555-92-1]

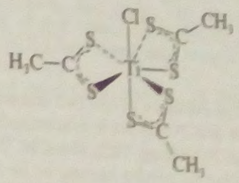
Frontas'ev, V.P. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1957, 113, 1073 (*thiourea adduct*)
Moeller, T. *et al, J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth, ir, adduct*)
Witt, J.R. *et al, J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Misra, S.N. *et al, J. Inorg. Nucl. Chem.*, 1963, **25**, 201 (*synth*)
Grigor'ev, A.I. *et al, Zh. Neorg. Khim.*, 1964, **9**, 1060; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 580 (*synth, ir*)
Hart, F.A. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 1605, 1825 (*adducts*)
Pospelova, L.A. *et al, Zh. Neorg. Khim.*, 1965, **10**, 1097; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1965, **10**, 594 (*synth, tga*)
Sadikov, G.G. *et al, Zh. Strukt. Khim.*, 1967, **8**, 551; *J. Struct. Chem. USSR (Engl. Transl.)*, 1967, **8**, 492 (*cryst struct*)
Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*)
Sakharova, Yu.G. *et al, Zh. Neorg. Khim.*, 1973, **18**, 656; 1978, **23**, 2543; 1979, **24**, 2969; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 343; 1978, **23**, 1407; 1979, **24**, 1652 (*uvvis, adducts, ir, tga*)
Batkibekova, M. *et al, Zh. Neorg. Khim.*, 1979, **24**, 2983; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1658 (*thermodyn*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. vol., 1984, **D5**, 31 (*rev*)

$C_6H_9ClS_6Ti$ IC-005036

Chlorotris(dithioacetato)titanium(*IV*)

Chlorotris[*ethane*(*dithioato-S,S′*)]*titanium*(IV), *10CI*

[74418-74-9]



M 356.8

Pentagonal bipyramidal at Ti. Synth. from $TiCl_4$ and the acid in Et_2O at −30°. V. air-sensitive solid.

Gastaldi, L. *et al, Cryst. Struct. Commun.*, 1980, **9**, 469 (*synth, cryst struct*)

$C_6H_9Cl_3CrN_3$ IC-005037

Trichlorotris(isocyanomethane)chromium, 9CI

Chromium(III)*chloride tris*(*methyl isocyanide*)

[58019-12-8]

$CrCl_3(CNMe)_3$

M 281.5

Stereochem. not reported. Green solid. Ir ν_{NMe} 2255 cm^{-1} (mull); μ_{eff} = 3.9μ_B.

Crociani, B. *et al, J. Organomet. Chem.*, 1975, **101**, C1 (*synth*)

$C_6H_9Cl_3MoN_3$ IC-005038

Tris(acetonitrile-*N*)trichloromolybdenum(*III*)

Molybdenum(III) *chloride tris*(*acetonitrile*)

[102977-17-3]

$MoCl_3(NCCH_3)_3$

M 325.4

mer-Octahedral geometry about Mo. Yellow cryst. + 1MeCN ($MeCN/Et_2O$).

[45047-76-5]

Roh, S.-Y. *et al, Inorg. Chem.*, 1986, **25**, 3105 (*cryst struct, synth*)

$C_6H_9Cl_3N_3Ru$ IC-005039

Tris(acetonitrile)trichlororuthenium(*III*), 9CI

Trichlorotris(*ethanenitrile*)*ruthenium*(III). *Ruthenium*(III) *chloride tris*(*acetonitrile*)

[45047-78-7]

$RuCl_3(NCCH_3)_3$

M 330.5
mer-Octahedral geometry.
Acetonitrile solvate: Prepd. by treating $[RuCl_3[SPh(CHMe_2)]_2(MeOH)]$ with MeCN. Red cryst. Mp 110° dec.

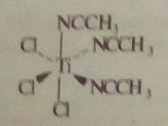
[21503-88-8]

Fr. Pat., 1 546 530, (1968); *CA*, **71**, 49350 (*use*)
UK Pat., 1 102 460, (1968); *CA*, **69**, 77513 (*use*)
Chatt, J. *et al*, *J. Chem. Soc. A*, 1971, 1380 (*synth, ir*)
Dehand, J. *et al*, *J. Chem. Res. (S)*, 1979, 155 (*synth*)
Eur. Pat., 72 435, (1983); *CA*, **98**, 199506 (*use*)

$C_6H_9Cl_3N_3Ti$ IC-005040

Tris(acetonitrile)trichlorotitanium(*III*), 11CI
Titanium(III) *chloride tris(acetonitrile)*

[18039-89-9]



fac-form

M 277.3
Octahedral. The existence of the two isomers is not well proven. The MeCN adduct is synthesised by dissolving $TiCl_3$ in MeCN yielding $TiCl_3.4MeCN$. $TiCl_3.3MeCN$ is then obt. either by careful heating or by evacuation at r.t. Constit. of olefin polym. catalyst.

fac-form [27183-96-6]
cis-form

mer-form [37580-88-4]
trans-form

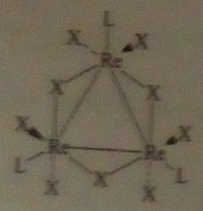
MeCN complex (1:1): [35835-55-3].
Dark blue solid. Paramagnetic; $\mu_{eff} = 1.75\mu_B$.

O'Brien, J.F. *et al*, *Inorg. Chem.*, 1970, **9**, 1000 (*esr, nmr, fac*-form)
Ostendorf, H.K., *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1972, **91**, 809 (*esr, us, mer*-form)
Zikmund, M. *et al*, *Chem. Zvesti*, 1979, **33**, 217; *CA*, **91**, 167707b (*synth*)
Czech. Pat., 181 979, (1980); *CA*, **94**, 122304p (*use*)
Mazo, G.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1986, **31**, 298 (*synth, deriv*)

$C_6H_9Cl_6N_3Re_3$ IC-005041

Tri-μ-chlorohexachlorotris(isocyanomethane) trirhenium(*III*), 11CI
Nonachlorotri(methyl isocyanide)trirhenium(III)

[89308-99-6]



L = CNMe, X = Cl

M 1000.8
Synth. from Re_2Cl_8 and MeNC in MeOH. Purple solid. Sol. CH_2Cl_2.

Monomer: Rhenium(III) *trichloride isocyanomethane*
$C_3H_3Cl_3NRe$ M 333.6

Unknown.

Cameron, C.J. *et al*, *J. Organomet. Chem.*, 1983, **255**, 345 (*synth, ir, uv, electrochem*)

$C_6H_9CrO_6$ IC-005042

Chromium(*III*) acetate

$Cr(OAc)_3$

M 229.1
May be identical to Hexakis-μ-acetatotriaqua-μ-oxotrichromium(*III*)(1+), IC-007853. Starting material.
Monohydrate: Commercially available. Grey-green powder or bluish green pasty mass. Sol. H_2O. May be identical to the trimer (q.v.).
Hexahydrate: Hexaaquachromium(3+) *triacetate*
Blue-violet needles. Sol. H_2O.

[1066-30-4]

Inorg. Synth., 1946, **2**, 203.
Brauer, G., *Handbook Prep. Inorg. Chem.*, 2nd Ed., Academic Press, N.Y., 1965-1971, **3**, 1373 (*synth, hexahydrate*)

$C_6H_9DyO_6$ IC-005043

Dysprosium(*III*) acetate
Dysprosium triacetate

[18779-07-2]

$Dy(OAc)_3$

M 339.6
Yellow solid. Sol. H_2O.
Tetrahydrate: [15280-55-4].
Yellow needles. Sol. H_2O; sl. sol. EtOH. Dec. at 120°. Loses H_2O on heating *in vacuo*.
Phen complex: Yellow cryst. Dec. at 270-274°.

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605.
Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9ErO_6$ IC-005044

Erbium(*III*) acetate
Erbium triacetate

[25519-10-2]

$Er(OAc)_3$

M 344.3
Pink solid. Sol. H_2O.
Tetrahydrate: [15280-57-6].
Pale pink or white cryst. Sol. H_2O. 9-Coord. Er in tricapped trigonal prismatic environment. Isomorphous with Gd analogue. Loses H_2O on heating *in vacuo*.
Phen complex: Cryst. Dec. at 267-270°.

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Grigor'ev, A.I. *et al*, *Zh. Neorg. Khim.*, 1964, **9**, 1060; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1964, **9**, 580 (*synth, ir*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605 (*adduct*)
Karraker, D.G. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*)
Ferraro, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 1495 (*ir*)
Petrov, K.I. *et al*, *Zh. Prikl. Spektrosk.*, 1970, **13**, 99; *J. Appl. Spectrosc. USSR (Engl. Transl.)*, 1970, **13**, 931 (*us-vis*)
Asianov, L.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1972, **205**, 343 (*cryst struct, us-vis*)

Batkibekova, M. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2983; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1658 (*therm props*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9EuO_6$ IC-005045

Europium(*III*) acetate
Europium triacetate

[1184-63-0]

$Eu(OAc)_3$

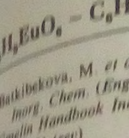
M 329.0
Colourless solid. Sol. H_2O.
Tetrahydrate: [37725-53-4].
Sol. H_2O, DMSO.
DMF complex: Mp 137-140°. Loses DMF *in vacuo* at 210°.
Tris-urea complex: [68462-09-9].
Colourless cryst. + $1.5H_2O$. Sol. H_2O.
Phen complex: Cryst. Dec. 268-272°.

[62667-64-5, 72555-96-5, 99646-38-5, 101953-41-7]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605 (*complex*)
Kleinermann, M. *et al*, *J. Chem. Phys.*, 1968, **49**, 3901 (*complex, fluorescence*)
Sakharova, Yu.G. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 2543; 1979, **24**, 2969; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 1407; 1979, **24**, 1652 (*urea complex, dga, dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9FeI_2O_3P$ IC-005046

Tricarbonyldiiodo(trimethylphosphine)iron, 8CI



abc-tricarbonyl-*de*-diiodo-*f*-phosphine-*form*

M 469.7

abc-Tricarbonyl-de-diiodo-f-phosphine-form [22624-27-7]
mono-cis,fac-*form*
Brown needles. μ 6.6 D.

alf-tricarbonyl-cd-diiodo-e-phosphine-form [62107-13-5]
mono-cis,mer-*form*
Brown prisms.

alf-tricarbonyl-ce-diiodo-d-phosphine-form [62075-78-9]
mono-trans,mer-*form*
Cryst.

Punkowski, M. *et al*, *J. Organomet. Chem.*, 1977, **125**, 231 (*synth, ir, nmr*)

$C_6H_9GaO_6$ IC-005047

Gallium(*III*) acetate
Gallium(III) *ethanoate. Triacetatogallium*

$Ga(OAc)_3$

M 246.8
Synth. from $GaCl_3$ + HOAc in Et_2O or from Ga + HOAc. Colourless moisture sensitive solid. Spar. sol. Et_2O, alcohols.

Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1964, **330**, 70; 1965, **337**, 142 (*synth*)

$C_6H_9GdO_6$ IC-005048

Gadolinium(*III*) acetate
Gadolinium triacetate

[31298-16-5]

$Gd(OAc)_3$

M 334.3
Colourless solid. Sol. H_2O.
Tetrahydrate: [73534-51-7]. *Bis-[μ-(acetato-O:O,O')tetrakis(acetato-O,O')tetraaquadigadolinium tetrahydrate, 10CI*
$C_6H_{17}GdO_{10}$ M 406.4
Colourless triclinic cryst. Sol. H_2O. 9-Coord. Gd is bound to 3 bidentate acetates, $2H_2O$ and one bridging acetate.
DMF complex: Sol. H_2O. Loses DMF *in vacuo* at 210°.
Phen complex: Cryst. Dec. at 265-268°.

[14432-01-0, 16056-77-2, 79464-08-7, 100587-93-7]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **16**, 1605 (*complex*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **24**, 637 (*synth*)
Kleinermann, M. *et al*, *J. Chem. Phys.*, 1968, **49**, 3901 (*complex*)
Favas, M.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 454 (*cryst struct, tetrahydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9Hg_2O_6^{\oplus}$ IC-005049

[μ-(Acetato-*O*:*O'*)]bis(acetato-*O*)dimercury(1+)
Tris(acetato)dimercury(1+)

$[Hg_2(OAc)_3]^{\oplus}$

M 578.3 (ion)
Nitrate: [122449-12-1]. *Acetato(nitrato-O)mercury mercuryacetate complex*
$C_6H_9Hg_2NO_9$ M 640.3
Formed from $Hg(NO_3)_2.H_2O$ in Ac_2O or $Ac_2O.AcOH$. Cryst. Cryst. struct. comprises $[HgOAc]^{\oplus}$, $NO_3^{\ominus}$ and $Hg(OAc)_2$ units.

Grdenic, D. *et al*, *Croat. Chim. Acta*, 1989, **62**, 27 (*synth, cryst struct*)

$C_6H_9HoO_6$ IC-005050

Holmium(*III*) acetate
Holmium triacetate

[25519-09-9]

$Ho(OAc)_3$

M 342.0
Yellow solid. Sol. H_2O.
Tetrahydrate: [15280-56-5].
Yellow cryst. Sol. AcOH. 9-Coord.; contains dimeric $Ho_2(OAc)_6(H_2O)_4$ units.
Phen complex: Cryst. Dec. at 261-263°.

[70457-40-8, 74392-05-5, 85077-86-7]

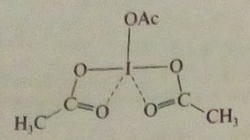
Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605 (*adduct*)
Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*)
Bats, J.W. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 1225 (*cryst struct*)
Batkibekova, M. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2983; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1658 (*thermodyn*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9IO_6$ IC-005051

Tris(acetato)iodine

Iodine(III) *triacetate. Acetic acid trianhydride with iodous acid* (H_3IO_3), *10CI, 9CI*

[56021-54-6]



M 304.0

Pentagonal planar struct. with 3 short (~215) and 2 long (~248 pm) I—O distances. Formed from I_2 + fuming HNO_3 + HOAc/Ac_2O. Colourless cryst.

Fichter, F. *et al*, *Helv. Chim. Acta*, 1928, **11**, 1256 (*synth*)
Birchall, T. *et al*, *Inorg. Chem.*, 1989, **28**, 636 (*synth, cryst struct, mössbauer*)

$C_6H_9InO_6$ IC-005052

Indium(*III*) acetate

Indium(III) *ethanoate. Tris(acetato)indium*

[40724-23-0]

$In(OAc)_3$

M 291.9

Synth. from $In(OH)_3$ and hot HOAc. White moisture sensitive needles (aq. HOAc). Mp 280° dec.

Bipy complex: [70279-27-5]. *Tris(acetato-O,O′)(2,2′-bipyridine-N,N′)indium*(III), *9CI*
$C_{16}H_{17}InN_2O_6$ M 448.1
Synth. from $In(OAc)_3$ and bipy in anhydrous HOAc. White cryst. (MeOH). 8-Coord. with all four ligands bidentate.

Phen complex: [70279-28-6]. *Tris(acetato-O,O′)(1,10-phenanthroline-N¹,N¹⁰)indium*(III), *9CI*
$C_{18}H_{17}InN_2O_6$ M 472.1
White cryst (MeOH). 8-Coord. with all four ligands bidentate.

Habeeb, J.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 243 (*synth, props, ir*)
Lindel, W. *et al*, *Z. Anorg. Allg. Chem.*, 1974, **408**, 167 (*ir*)
Preut, H. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **450**, 120 (*cryst struct, complexes*)

$C_6H_9LaO_6$ IC-005053

Lanthanum(*III*) acetate

Lanthanum triacetate

[31396-47-1]

$La(OAc)_3$

M 316.0

White solid. Sol. C_5H_5N. Dec. to La_2O_3 at 760°.

Monohydrate: [17829-81-1].
Colourless cryst. 9-Coord. tricapped trig. prism. Sesquihydrate and pentahydrate also reported.

1.5 Hydrate: Colourless cryst. Sol. H_2O.

Tris-urea complex: [41579-89-9].
Colourless cryst. + $1.5H_2O$. Sol. H_2O. Mp 139°.

Thiourea complex: Colourless cryst. + $2H_2O$. Mp 258-260°.

[917-70-4, 72555-91-0, 100587-90-4]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Misra, S.N. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **25**, 201 (*synth*)
Grigor'ev, A.I. *et al*, *Zh. Neorg. Khim.*, 1964, **9**, 1060; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 580 (*synth, ir*)
Frontas'ev, V.P. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 990 (*thiourea deriv*)
Kleinermann, M. *et al*, *J. Chem. Phys.*, 1968, **49**, 3901 (*deriv*)
Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*)
Ferraro, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 1495 (*ir*)
Sakkarova, Yu.G. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 2543; 1979, **24**, 2969; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 1407; 1979, **24**, 1652 (*synth, ir, tga, dta*)
Batkibekova, M. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2983; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1658 (*thermodyn*)
Antsyshkina, A.S. *et al*, *Dokl. Akad. Nauk Azerb. SSR*, 1980, **36**, 47; *CA*, **96**, 13893 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9LuO_6$ IC-005054

Lutetium(*III*) acetate

Lutetium triacetate

[18779-08-3]

$Lu(OAc)_3$

M 352.1

Colourless solid. Sol. H_2O.

Tetrahydrate: [15280-59-8].
Colourless cryst.

Phen complex: Cryst. Dec. at 277-280°.

Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605 (*deriv*)
Batkibekova, M. *et al*, *Zh. Neorg. Khim.*, 1979, **14**, 2983; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **14**, 1658 (*thermodyn*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9NdO_6$ IC-005055

Neodymium(*III*) acetate

Neodymium triacetate

[6192-13-8]

$Nd(OAc)_3$

M 321.3

Red solid.

▷ AI9700000.

1.5 Hydrate: Red solid. Sol. H_2O.

Tetrahydrate: [50484-87-2].
Red cryst. Sol. H_2O.

DMF complex: Red cryst. Mp 151-155°. Loses DMF *in vacuo* at 210°.

Tris-urea complex: [41579-92-4].
Red cryst. + $1.5H_2O$. Sol. H_2O. Mp 135.5-136.5°.

Thiourea complex: Red cryst. + $1H_2O$.

2,2′-Bipy complex: Cryst. Mp 250-260°.

Phen complex: Cryst. Dec. at 300-310°.

[16648-22-9, 16922-03-5, 25721-95-3, 61907-70-8, 72555-94-3]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605, 1825 (*derivs*)
Mehrotra, R.C. *et al*, *Indian J. Chem.*, 1966, **43**, 61 (*synth*)
Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir, uv-vis*)
Grigor'ev, A.I. *et al*, *Zh. Neorg. Khim.*, 1969, **9**, 1060; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 580 (*synth, ir*)
Batkibekova, M. *et al*, *Zh. Fiz. Khim.*, 1976, **50**, 1914 (*thermodyn*)
Sakharova, Yu.G. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 2543; 1979, **24**, 2969; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 1407; 1979, **24**, 1652 (*urea derivs, tga, dta, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9NiO_6P$ IC-005056

Tricarbonyl(trimethyl phosphite-*P*)nickel, 9CI

(Trimethyl phosphite)nickel tricarbonyl.
Tricarbonyl(phosphorous acid)nickel trimethyl ester, 8CI

[17099-58-0]

$Ni(CO)_3P(OMe)_3$

M 266.7

Catalyst for dimerisation of pentyne, ethene and cycloalkadienes. Cryst. (pentane or MeOH).

Bignorgne, M., *Bull. Soc. Chim. Fr.*, 1960, 1986 (*synth, ir*)
Bouquet, G. *et al*, *J. Mol. Struct.*, 1968, **1**, 211 (*ir, raman*)
Mathieu, R. *et al*, *Inorg. Chem.*, 1970, **9**, 2030 (*nmr*)
Bodner, G.M., *Inorg. Chem.*, 1975, **14**, 1932 (*nmr*)

$C_6H_9NpO_8^{\ominus}$ IC-005057

Triacetatodioxoneptunate(*VI*)(1−)

$[NpO_2(OAc)_3]^{\ominus}$

M 446.1 (ion)

8-Coordinate hexagonal bipyramidal struct. with axial oxide ligands.

Na salt: [19663-31-1].
Pale green-yellow cryst. (pink by reflected light, green by transmitted light). Sol. H_2O. Ir $\nu_{Np=O}$ 934 cm^{-1}. Isomorphous with U, Pu, Am analogues.

Cs salt: [18770-97-3].
Tetragonal pyramidal cryst. Sol. H_2O.

[81446-17-5]

Zachariasen, W.H., *Acta Crystallogr.*, 1949, **2**, 388; 1954, **7**, 795 (*struct*)
Vdovenko, V.M. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1973, **209**, 352 (*synth, ir*)
Vdovenko, V.M. *et al*, *Radiokhimiya*, 1974, **16**, 716 (*ir*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1281 (*synth*)
Gorshkov, N.G. *et al*, *Sov. Radiochem.* (*Engl. Transl.*), 1980, **22**, 325 (*synth, uv-vis*)
Glebov, V.A., *Koord. Khim.*, 1981, **7**, 894 (*pe*)
Alcock, N.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 33 (*cryst struct*)

$C_6H_9O_3S_6Sb$ IC-005058

Tris(*O*-methyl carbonodithioato-*S,S′*)antimony, 11Cl, 9Cl

Tris(O-*methyl dithiocarbonato*)*antimony. Tris*(O-*methyl xanthato*)*antimony. Antimony tri*(*methyl xanthate*)

[41322-38-7]

$Sb[SC(S)OMe]_3$

M 443.2

Cryst. (CH_2Cl_2). Mp 114-115°. Loosely held dimeric struct.

Khwaja, M.H. *et al*, *Anal. Chim. Acta*, 1973, **64**, 9 (*synth, props*)
Snow, M.R. *et al*, *Aust. J. Chem.*, 1987, **40**, 743 (*cryst struct*)

$C_6H_9O_6Pr$ IC-005059

Praseodymium(*III*) acetate

Praseodymium triacetate

[6192-12-7]

$Pr(OAc)_3$

M 318.0

Green solid. Sol. H_2O. Dec. > 270°; Pr_6O_{11} formed at 790°.

Monohydrate: Light green cryst. Contains 9-coord. Pr with bridging acetates.

1.5 Hydrate: Green needles. Sol. H_2O. Loses H_2O at 100°, completely dehyd. at 230°. Dec. >270°.

DMF complex: Mp 151-155°. Loses DMF *in vacuo* at 210°.

Tris-urea complex: [41579-91-3].
Green cryst. + $1.5H_2O$. Sol. H_2O. Mp 138-139.5°.

Thiourea complex: Green cryst. Sol. H_2O. Mp 197-198°.

Phen complex: Green cryst. Dec. at 270-300°.

2,2′-Bipy complex: Green cryst. Dec. at 250-260°.

[17829-83-3, 71546-14-0, 72555-93-2]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605, 1825 (*derivs*)
Frontas'ev, V.P. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 990 (*synth, thiourea deriv*)
Mehrotra, R.C. *et al*, *J. Indian Chem. Soc.*, 1966, **43**, 61 (*synth*)
Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*)
Sakharova, Yu.G. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 2543; 1979, **24**, 2969; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 1407; 1979, **24**, 1652 (*urea deriv, tga, dta, ir*)
Manabe, K. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1983, 450; *CA*, **98**, 209096 (*thermal anal, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39 *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)
Ganapathy, S. *et al*, *J. Am. Chem. Soc.*, 1990, **108**, 12 (*cryst struct*)
Hehlen, M.P. *et al*, *Inorg. Chem.*, 1991, **30**, 2273 (*synth, uv-vis, raman*)

$C_6H_9O_6Rh_2^{\oplus}$ IC-005060

Tri-μ-acetatodirhodium(*II*)(1+)

Tris[*μ*-(*acetato*-O:O′)]*dirhodium*(II)(*1+*), *10CI*

[72451-78-6]

$[Rh_2(OAc)_3]^{\oplus}$

M 382.9 (ion)

Prepd. from $Rh_2(OAc)_4$ in aq. soln. of a non complexing acid such as trifluoromethylsulfonic, perchloric or *p*-toluenesulfonic acid. Present as cation in soln. and not isol.

Wilson, C.R. *et al*, *Inorg. Chem.*, 1975, **9**, 2276 (*synth, uv*)

$C_6H_9O_6Sc$ IC-005061

Scandium(*III*) acetate

Scandium triacetate

[3804-23-7]

$Sc(OAc)_3$

M 222.0

Polymeric struct. with octahedral Sc. Colourless solid. Sol. H_2O. Dec. at >285°.

Monohydrate: Colourless cryst. Loses H_2O ~ 150°.

Sterba-Böhm, J.S. *et al*, *Collect. Czech. Chem. Commun.*, 1935, **7**, 57 (*synth*)
Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1963, **325**, 67 (*synth*)
Komissarova, L.N. *et al*, *Izv. Akad. Nauk SSSR Neorg. Mat.*, 1968, **4**, 1094; *Inorg. Materials* (*Engl. Transl.*), 1968, **4**, 962 (*tga*)
Porai-Koshits, M.A. *et al*, *Kristallografiya*, 1971, **16**, 1195; *Sov. Phys. Crystallogr.* (*Engl. Transl.*), 1971, **16**, 1047 (*cryst struct*)
Smolyakova, K.E. *et al*, *Tr. Tomsk. Gos. Univ.*, 1973, **237**, 143; *CA*, **80**, 59389 (*hydrate*)
Fuchs, R. *et al*, *Z. Naturforsch., B*, 1984, **39**, 1662 (*synth, cryst struct*)

$C_6H_9O_6Sm$ IC-005062

Samarium(*III*) acetate

Samarium triacetate

[10465-27-7]

$Sm(OAc)_3$

M 327.4
Yellow solid. Sol. H_2O.
▷ AJ3890000.
Tetrahydrate: [15280-52-1].
Yellow cryst. Sol. H_2O.
DMF complex: Yellow solid. Mp 137-140°. Loses DMF *in vacuo* at 210°.
Tris-urea complex: [41579-93-5].
Yellow cryst. + $1.5H_2O$. Sol. H_2O.
Thiourea complex: Yellow cryst. + $0.5H_2O$. Sol. H_2O.
Phen complex: Yellow cryst. Dec. at 286-290°.

[17829-87-7, 72555-95-4, 100587-91-5]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605 (*adduct*)
Frontas'ev, V.P. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 990 (*thiourea deriv*)
Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*;1Sakharova, Yu.G. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 2543; 1979, **24**, 2969; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 1407; 1979, **24**, 1652 (*urea adduct, ir, tga, dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9O_6Tb$ IC-005063

Terbium(*III*) acetate
Terbium triacetate
[25519-07-7]

$Tb(OAc)_3$

M 336.0
Pale pink solid. Sol. H_2O.
Tetrahydrate: [15280-54-3].
Pale pink solid. Sol. H_2O.
Phen complex: Cryst. Dec. at 270-275°.

[85077-88-9, 100587-92-6]

Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605 (*adduct*)
Kleinermann, M. *et al*, *J. Chem. Phys.*, 1968, **49**, 3901 (*adduct, fluorescence*)
Ferraro, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 1495 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39 *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)

$C_6H_9O_6Tl$ IC-005064

Thallium(*III*) acetate
Thallium(III) *ethanoate. Triacetatothallium*
[2570-63-0]

$Tl(OAc)_3$

M 381.5
Monoclinic; Tl is coordinated by three chelate acetate groups with two further longer Tl—O bonds leading to TlO_6 chain formation. Synth. from Tl_2O_3 and boiling AcOH. Strong Lewis acid. Friedel-Crafts catalyst; mild oxidising agent; with Br_2 selectively brominates aromatic compds. in the *p*-position. White platelets, rapidly hydrol.
▷ V. toxic.

Kochi, J.K. *et al*, *J. Org. Chem.*, 1968, **33**, 75 (*synth*)
Taylor, E.C. *et al*, *Acc. Chem. Res.*, 1970, **3**, 338 (*reaction*)
Faggiani, R. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 2845; 1982, **38**, 2473 (*struct*)

$C_6H_9O_6Tm$ IC-005065

Thulium(*III*) acetate
Thulium triacetate
[39156-80-4]

$Tm(OAc)_3$

M 346.0
Green solid. Sol. H_2O.
Tetrahydrate: [34431-47-5].
Green cryst. Sol. H_2O.
Phen complex:
$C_{18}H_{17}N_2O_6Tm$ M 526.2
Cryst. Dec. at 275-280°.

Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605 (*complex*)
Petrov, K.I., *Zh. Prikl. Spektrosk.*, 1971, **15**, 296; *J. Appl. Spectrosc. USSR* (*Engl. Transl.*), 1971, **15**, 1058 (*uv-vis*)
Batkibekova, M. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2983; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1658 (*thermodyn*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1984, **D5**, 31 (*rev, bibl*)

$C_6H_9O_6Y$ IC-005066

Yttrium(*III*) acetate
Yttrium triacetate
[23363-14-6]

$Y(OAc)_3$

M 266.0
White solid. Sol. H_2O.
Tetrahydrate: [85949-60-6].
Colourless cryst. Sol. H_2O.

[26908-14-5]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Grigor'ev, A.I. *et al*, *Zh. Neorg. Khim.*, 1964, **9**, 1060; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 580 (*synth, ir*)
Grigor'ev, A.I. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1969, **10**, 43.
Ferraro, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 1495 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No 39 *Suppl. No.*, 1984, D5, 31 (*rev*)

$C_6H_9O_6Yb$ IC-005067

Ytterbium(*III*) acetate
Ytterbium triacetate
[31298-17-6]

$Yb(OAc)_3$

M 350.1
White solid. Sol. H_2O.
Tetrahydrate: [15280-58-7].
Colourless cryst. Sol. H_2O. Loses H_2O on heating to 70°. Dec. >300° to YbO(OAc) and Yb_2O_3.
2,2'-Bipy complex:
$C_{16}H_{17}N_2O_6Yb$ M 506.3
Cryst. Dec. at 240-245°.
Phen complex:
$C_{18}H_{17}N_2O_6Yb$ M 530.3
White cryst. Dec. at 288-290°.

[20981-49-1]

Moeller, T. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **15**, 259 (*synth*)
Witt, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1963, **24**, 637 (*synth*)
Grigorev, A.I. *et al*, *Zh. Neorg. Khim.*, 1964, **9**, 1060; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 580 (*synth, ir*)
Hart, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 1605, 1825 (*complex*)

Karraker, D.G., *J. Inorg. Nucl. Chem.*, 1969, **31**, 2815 (*synth, ir*)
Batkibekova, M. *et al*, *Zh. Neorg. Khim.*, 1979, **24**, 2983; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1979, **24**, 1658 (*thermodyn*)
Gmelin Handbook Inorg. Chem., Syst No. 39. *Suppl. Vol.*, 1984, **D5**, 31 (*rev*)
Ogawa, M. *et al*, *Kogei Daigaku Kogakubu. Kiyo Tokyo*, 1984, **7**, 41 (*synth, dta, tga*)

$C_6H_9O_6Zn^{\ominus}$ IC-005068

Tris(acetato-*O*)zincate(1−)
[18747-53-0]

$[Zn(OAc)_3]^{\ominus}$

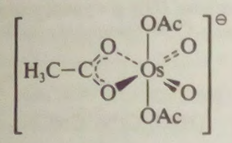
M 242.5 (ion)
Li salt: [41743-14-0].
Solid.

[46140-22-1]

Warnke, Z. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1969, **43**, 1939 (*stability const, anion*)
Pavlov, V.L. *et al*, *CA*, 1973, **78**, 128969 (*synth, salts*)
Sawada, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2282 (*stability const*)
Kuznetsov, Yu.M. *et al*, *Deposited Doc.*, VINITI, 1978, 1816-78; *CA*, 1979, **91**, 182183 (*cryst struct*)
Yang, M.M. *et al*, *Geochim. Cosmochim. Acta*, 1989, **53**, 319 (*raman*)

$C_6H_9O_8Os^{\ominus}$ IC-005069

Tris(acetato)dioxoosmate(*VI*)(1−)
Bis(acetato-O)(*acetato*-O,O')*dioxoosmate*(VI)(*1−*), *11CI*



M 399.3 (ion)
K salt: [85651-46-3].
Obt. by reaction of $K_2[OsO_2(OMe)_4]$ with glacial AcOH.
Dark blue solid.
K salt, bis-HOAc solvate: [85651-47-4].
Deep blue air-sensitive cryst. (AcOH).

[37209-95-3]

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1449 (*synth, ir*)
Behling, T. *et al*, *Polyhedron*, 1982, **1**, 840 (*cryst struct*)

$C_6H_9O_8Pu^{\ominus}$ IC-005070

Tris(acetato-*O*)dioxoplutonate(*VI*)(1−), 11CI
Plutonyl acetate(*1−*)
[22992-42-3]

$[PuO_2(OAc)_3]^{\ominus}$

M 448.1 (ion)
Insol. alkali metal salts have been used in Pu purif.
Na salt: [12012-89-4].
$C_6H_9NaO_8Pu$ M 471.1
Pink cryst. Sl. sol. H_2O. Paramagnetic; μ_{eff} = 2.83 μ_B. Probably 8-coordinate with bidentate nitrates.
Cs salt: [18307-91-0].
$C_6H_9CsO_8Pu$ M 581.0
Pink cryst.

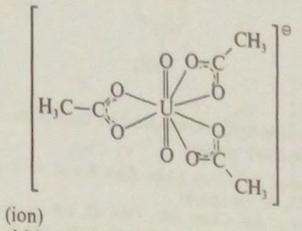
[18129-45-8]

Dawson, J.K. *et al*, *J. Chem. Soc.*, 1952, 2705 (*synth*)
Zachariasen, W.H., *Acta Crystallogr.*, 1954, **7**, 795; 1959, **12**, 526 (*struct*)

Jones, C.H., *J. Chem. Phys.*, 1955, **23**, 2105 (*synth, ir*)
Ryan, J.L. *et al*, *Adv. Chem. Ser.*, 1967, **71**, 335 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, **C4**, 235 (*rev*)
Vdovenko, V.M. *et al*, *Radiokhimiya*, 1974, **16**, 716 (*ir*)

$C_6H_9O_8U^{\ominus}$ IC-005071

Tris(acetato)dioxouranate(*VI*)(1−)
Uranyl acetate(*1−*)



M 447.1 (ion)
Hexagonal bipyramidal struct. with U=O 176, U—O 246 pm (Na salt).
Na salt: [17712-38-8].
Yellow solid. Ir $\nu_{U=O}$ 918 (932) cm^{-1}. Dec. at 250-300°.
NH_4 salt: [15746-17-5].
Air-stable yellow needles. Sol. H_2O, HOAc, EtOH. Ir $\nu_{U=O}$ 951, 928 cm^{-1}.
Ethylenediammonium(*2+*) *salt* (*2:1*): [104067-50-7].
Green-yellow cryst. Sol. H_2O. Dec. >200° to $UO_2(OAc)_2.\frac{1}{2}$(en) then to UO_3. Ir $\nu_{U=O}$ 942, 930 cm^{-1}.
Tetrakis(*decyl*)*ammonium salt:* Viscous yellow-green liq.

Zachariasen, W.H. *et al*, *Acta Crystallogr.*, 1959, **12**, 526 (*cryst struct*)
Volod'ko, L.V. *et al*, *Zh. Prikl. Spektrosk.*, 1965, **3**, 65; *CA*, 1966, **64**, 2866.
Ohwada, K., *Spectrochim. Acta, Part A*, 1968, **24**, 595 (*ir*)
Volod'ko, L.V. *et al*, *Zh. Neorg. Khim.*, 1968, **13**, 297; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1968, **13**, 154 (*ir*)
Vdovenko, V.M. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1973, **209**, 352 (*ir*)
Denning, R.G. *et al*, *Mol. Phys.*, 1979, **37**, 1089 (*synth, uv*)
Templeton, D.H. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 1439 (*cryst struct*)
Charpin, P. *et al*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1985, **82**, 925 (*exafs*)
Dubrovin, A.V. *et al*, *Radiokhimiya*, 1986, **28**, 152; *Sov. Radiochem.* (*Engl. Transl.*), 1986, **28**, 135 (*synth, ir*)
Santalova, N.A. *et al*, *Radiokhimiya*, 1986, **28**, 162; *Sov. Radiochem.* (*Engl. Transl.*), 1986, **28**, 139 (*synth, ir*)

$C_6H_{10}AuN_2^{\oplus}$ IC-005072

Bis(isocyanoethane)gold(1+)
Bis(ethyl isocyanide)gold(*1+*)
[82582-20-5]

$[Au(CNEt)_2]^{\oplus}$

M 307.1 (ion)
Perchlorate:
$C_6H_{10}AuClN_2O_4$ M 406.5
Cryst. (Me_2CO/Et_2O). Sol. Me_2CO.

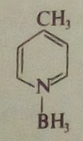
Chastain, S.K. *et al*, *Inorg. Chem.*, 1982, **21**, 3717 (*synth, mech*)

$C_6H_{10}BN$ IC-005073

Trihydro(4-methylpyridine)boron, 10CI

Borane 4-methylpyridine. 4-Methylpyridine compd. with borane(1:1), 9CI. 4-Picoline compd. with BH_3

[3999-39-1]



M 106.9

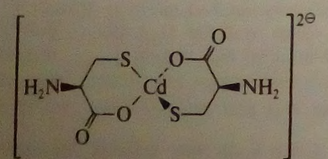
Used in photographic direct-positive emulsions. Shows antiflammatory activity.

Bigot, J.A. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1957, **76**, 996 (*synth*)
Brey, W.S. *et al, Adv. Chem. Ser.*, 1964, **42**, 100 (*nmr*)
Hoffmann, R., *J. Chem. Phys.*, 1964, **40**, 2474 (*struct*)
Mathur, M.A. *et al, Inorg. Chem.*, 1980, **19**, 887.
U.S. Pat., 4 312 989, (1982); *CA*, **97**, 85322g (*use*)

$C_6H_{10}CdN_2O_4S_2^{2\ominus}$ IC-005074

Bis[L-cysteinato(2−)-*N,S*]cadmate(2−)

(R)-form



M 350.6 (ion)

Di-H compd.: [57407-88-2].

Obt. from cysteine hydrochloride, Cd_2SO_4 and NaOH in H_2O. Cryst. + $2H_2O$ (H_2O). Insol. H_2O, EtOH, Et_2O; sol. acids. Stable to 150°; dehydration of dihydrate occurs at 150°. $H^{\oplus}$ are located on NH_2.

Zegzhda, G.D. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 1289 (*stab const, synth, ir*)
Zegzhda, G.D. *et al, Koord. Khim.*, 1976, **2**, 1031 (*synth, ir, pmr*)

$C_6H_{10}CdO_2S_4$ IC-005075

Bis(*O*-ethyldithiocarbonato-*S,S'*)cadmium

Bis(O-ethylcarbonodithioato-S,S')cadmium, 9CI. Bis(ethylxanthato)cadmium

$Cd[SC(S)OEt]_2$

M 354.8

Cryst.

Iimura, Y. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 2271 (*cryst struct*)

$C_6H_{10}CdO_4$ IC-005076

Cadmium propanoate

Cadmium propionate. Di(propionato)cadmium

[16986-83-7]

$Cd(OOCCH_2CH_3)_2$

M 258.5

Cryst. Dec. on heating to CdO.

Filipovic, I. *et al, Croat. Chim. Acta*, 1970, **42**, 541 (*stability const*)
Panevchuk, V.V. *et al, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1984, **27**, 677; 1985, **28**, 106 (*powder struct, thermal dec*)

$C_6H_{10}ClO_5Ta$ IC-005077

Chlorooxobis(propanoato-*O*)tantalum(*V*), 11CI

[100072-33-1]

$(H_3CCH_2COO)_2TaOCl$

M 378.5

Synth. from $TaCl_5$ and propanoic anhydride. Dec. by moist air. Ir ν_{TaO} 950 cm^{-1}.

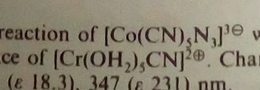
Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1985, **24**, 761 (*synth, ir*)

$C_6H_{10}Cl_3HfNS_2$ IC-005078

Trichloro(cyclopentylcarbamodithioato-*S,S'*)hafnium(*IV*), 11CI

Trichloro(cyclopentyldithiocarbamato)hafnium(IV)

[82428-97-5]



M 445.1

Synth. by heating under reflux equimolar quantities of $HfCl_4$ and Na salt of ligand in CH_2Cl_2. Reddish-brown moisture sensitive solid. Sol. CH_2Cl_2, $CHCl_3$, CCl_4, C_6H_6; insol. hydrocarbon solvs. Mp 140° dec.

Kumar, S. *et al, Indian J. Chem., Sect. A*, 1982, **21**, 182 (*synth, magnetism, ir, pmr*)

$C_6H_{10}CoCrN_6O_5$ IC-005079

[Pentaaquachromium(*III*)]-μ-cyano[pentacyanocobalt(*III*)]

Pentaaqua[μ-(cyano-C:N)][pentakis(cyano-C)cobalt]chromium, 10CI

[67870-85-3]

$(H_2O)_5CrNCCo(CN)_5$

M 357.1

Characterised in soln. Synth. from slow reaction of $[Cr(H_2O)_6]^{3\oplus}$ with $[Co(CN)_6]^{3\ominus}$. λ_{max} 560 nm (ε 16.2), 401 (ε 20.1), 310 (ε 218).

Gaswick, D. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 437 (*synth, uv-vis, isomer*)

$C_6H_{10}CoCrN_6O_5$ IC-005080

[Pentaaquachromium(*III*)]-μ-isocyano[pentacyanocobalt(*III*)]

Pentaaqua[μ-(cyano-N:C)][pentakis(cyano-C)cobalt]chromium

[67870-86-4]

$(H_2O)_5CrCNCo(CN)_5$

M 357.1

Made by rapid reaction of $[Co(CN)_5N_3]^{3\ominus}$ with nitrous acid in presence of $[Cr(OH_2)_5CN]^{2\oplus}$. Characterised in soln. λ_{max} 552 (ε 18.3), 347 (ε 231) nm.

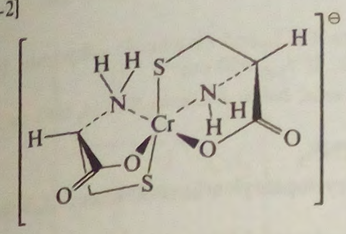
Gaswick, D. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 437 (*synth, uv-vis, isom*)

$C_6H_{10}CrN_2O_4S_2^{\ominus}$ IC-005081

Bis[L-cysteinato(2−)-*N,O,S*]chromate(*III*)(1−), 11CI, 10CI

(R)(R)-form

[91264-49-2]



M 290.2 (ion)

Cr in sl. distorted octahedral coord.

Na salt: [62126-04-9].

Blue cryst. + $2H_2O$.

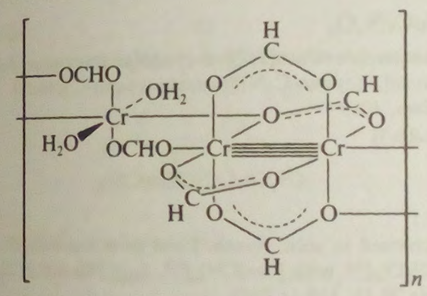
[91264-51-6, 100897-99-2]

de Meester, P. *et al, Inorg. Chem.*, 1977, **16**, 1494 (*cryst struct*)
Cooper, J.A. *et al, Inorg. Chim. Acta*, 1984, **92**, 23 (*synth*)
Abdullah, M. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 2085 (*synth, uv, cd*)

$C_6H_{10}Cr_3O_{14}$ IC-005082

Diaquahexakis(formato)trichromium(*II*)

[64611-48-9]



M 462.1

Struct. comprises infinite chains of alternating monomeric and dimeric units; the latter contain Cr≡Cr of 245.1 pm; the former have tetragonally distorted octahedral coord. Red needles (H_2O).

Cotton, F.A. *et al, Inorg. Chem.*, 1978, **17**, 176 (*cryst struct, synth*)

$C_6H_{10}CuO_4$ IC-005083

Copper(*II*) propanoate

Cupric propionate. Dipropanoatocopper

As Tetrakis[μ-(acetato-*O:O'*)]dicopper, IC-005990 with

$L = OH_2$, $R = CH_2CH_3$

M 209.6

Exists as dimeric hydrate.

Diaquatetrakis[μ-(propanoato-O:O')]dicopper [36539-04-5]

Cupric propanoate monohydrate. Aquadi(propionato-O:O')copper dimer

$C_{12}H_{24}Cu_2O_{10}$ M 455.4

Antiferromagnetic interactions between Cu atoms, Cu—Cu 257.5, Cu—OC 195 pm. Dark-green cryst. Sol. H_2O, dioxan, C_6H_6; sl. sol. $CHCl_3$.

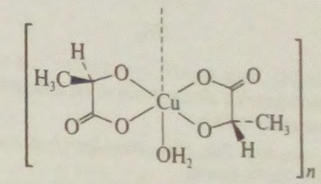
Martin, R.L. *et al, J. Chem. Soc.*, 1957, 2545 (*synth, magnetism*)
Doedens, R.J., *Prog. Inorg. Chem.*, 1976, **21**, 209 (*rev*)
Petrenko, P.A. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1985, **282**, 1375 (*cryst struct*)
Battaglia, L.P. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 1653 (*synth, esr, vis, ir, thermogravimetry, cryst struct*)
Kiosse, G.A. *et al, Kristallografiya*, 1987, **32**, 1277 (*cryst struct, esr*)

$C_6H_{10}CuO_6$ IC-005084

Aquabis(DL-lactato)copper(*II*)

Aquabis(2-hydroxypropanoato-O^1,O^2)copper, 11CI

[16039-52-4]



M 241.6

Approx. octahedral Cu. The sixth coordination site is occupied by a carboxy-oxygen from a neighbouring complex. Bactericide; fading inhibitor; used in corrosion resistant concrete and in dentrifice compositions. Efflorescent blue cryst. + $\frac{1}{2}H_2O$. Forms various hydrates.

[16039-52-4, 25215-50-3, 57628-78-1, 62482-70-6]

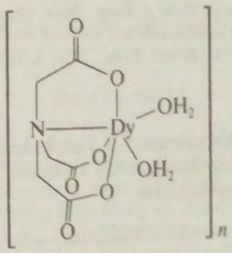
Prout, C.K. *et al, J. Chem. Soc. A*, 1968, 2791 (*cryst struct, synth*)
Dawson, K. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1509 (*esr*)
Warnke, Z. *et al, Pol. J. Chem. (Rocz. Chem.)*, 1973, **47**, 467; *CA*, **79**, 24045a (*props*)
Kharitonova, R.I. *et al, Koord. Khim.*, 1976, **2**, 1546 (*ir*)
Fogel, N. *et al, J. Chem. Soc., Faraday Trans. 2*, 1985, **81**, 21 (*esr*)

$C_6H_{10}DyNO_8$ IC-005085

Diaqua(nitrilotriacetato)dysprosium(*III*)

Diaqua[N,N'-bis(carboxymethyl)glycinato(3−)-N,O,O',O'']dysprosium(III), *9CI. (Nitrilotriacetato)diaquodysprosium*(III)

[37336-72-4]



M 386.6

8-Coord. struct. with bridging nitrilotriacetato groups. Lilac cryst. $+2H_2O$.

Fitch, F.T. *et al, Can. J. Chem.*, 1951, **29**, 363 (*use*)
Mitrofanova, N.D. *et al, Zh. Neorg. Khim.*, 1962, **7**, 1049; 1964, **9**, 320; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 539; 1964, **9**, 174 (*synth*)
Martin, L.L. *et al, Inorg. Chem.*, 1972, **11**, 2789 (*cryst struct*)

$C_6H_{10}FeO_6$ IC-005086

Ferrous lactate

Iron(II) *2-hydroxypropanoate. Iron*(II) *lactate*

[5905-52-2]

$Fe[OOCCH(OH)CH_3]_2$

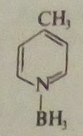
M 233.9

$C_6H_{10}BN$ IC-005073

Trihydro(4-methylpyridine)boron, 10CI

Borane 4-methylpyridine. 4-Methylpyridine compd. with borane(1:1), 9CI. 4-Picoline compd. with BH_3

[3999-39-1]



M 106.9

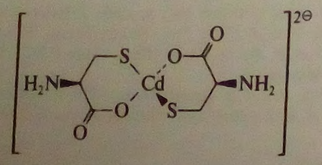
Used in photographic direct-positive emulsions. Shows antiflammatory activity.

Bigot, J.A. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1957, **76**, 996 (*synth*)
Brey, W.S. *et al, Adv. Chem. Ser.*, 1964, **42**, 100 (*nmr*)
Hoffmann, R., *J. Chem. Phys.*, 1964, **40**, 2474 (*struct*)
Mathur, M.A. *et al, Inorg. Chem.*, 1980, **19**, 887.
U.S. Pat., 4 312 989, (1982); *CA*, **97**, 85322g (*use*)

$C_6H_{10}CdN_2O_4S_2^{2\ominus}$ IC-005074

Bis[L-cysteinato(2−)-*N*,*S*]cadmate(2−)

(R)-form



M 350.6 (ion)

Di-H compd.: [57407-88-2].

Obt. from cysteine hydrochloride, Cd_2SO_4 and NaOH in H_2O. Cryst. + $2H_2O$ (H_2O). Insol. H_2O, EtOH, Et_2O; sol. acids. Stable to 150°; dehydration of dihydrate occurs at 150°. $H^{\oplus}$ are located on NH_2.

Zegzhda, G.D. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 1289 (*stab const, synth, ir*)
Zegzhda, G.D. *et al, Koord. Khim.*, 1976, **2**, 1031 (*synth, ir, pmr*)

$C_6H_{10}CdO_2S_4$ IC-005075

Bis(*O*-ethyldithiocarbonato-*S*,*S*′)cadmium

Bis(O-ethylcarbonodithioato-S,S′)cadmium, 9CI. Bis(ethylxanthato)cadmium

$Cd[SC(S)OEt]_2$

M 354.8

Cryst.

Iimura, Y. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 2271 (*cryst struct*)

$C_6H_{10}CdO_4$ IC-005076

Cadmium propanoate

Cadmium propionate. Di(propionato)cadmium

[16986-83-7]

$Cd(OOCCH_2CH_3)_2$

M 258.5

Cryst. Dec. on heating to CdO.

Filipovic, I. *et al, Croat. Chim. Acta*, 1970, **42**, 541 (*stability const*)
Panevchuk, V.V. *et al, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1984, **27**, 677; 1985, **28**, 106 (*powder struct, thermal dec*)

$C_6H_{10}ClO_5Ta$ IC-005077

Chlorooxobis(propanoato-*O*)tantalum(*V*), 11CI

[100072-33-1]

$(H_3CCH_2COO)_2TaOCl$

M 378.5

Synth. from $TaCl_5$ and propanoic anhydride. Dec. by moist air. Ir ν_{TaO} 950 cm^{-1}.

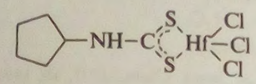
Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1985, **24**, 761 (*synth, ir*)

$C_6H_{10}Cl_3HfNS_2$ IC-005078

Trichloro(cyclopentylcarbamodithioato-*S*,*S*′)hafnium(*IV*), 11CI

Trichloro(cyclopentyldithiocarbamato)hafnium(IV)

[82428-97-5]



M 445.1

Synth. by heating under reflux equimolar quantities of $HfCl_4$ and Na salt of ligand in CH_2Cl_2. Reddish-brown moisture sensitive solid. Sol. CH_2Cl_2, $CHCl_3$, CCl_4, C_6H_6; insol. hydrocarbon solvs. Mp 140° dec.

Kumar, S. *et al, Indian J. Chem., Sect. A*, 1982, **21**, 182 (*synth, magnetism, ir, pmr*)

$C_6H_{10}CoCrN_6O_5$ IC-005079

[Pentaaquachromium(*III*)]-μ-cyano[pentacyanocobalt(*III*)]

Pentaaqua[μ-(cyano-C:N)][pentakis(cyano-C)cobalt]chromium, 10CI

[67870-85-3]

$(H_2O)_5CrNCCo(CN)_5$

M 357.1

Characterised in soln. Synth. from slow reaction of $[Cr(H_2O)_6]^{3\oplus}$ with $[Co(CN)_6]^{3\ominus}$. λ_{max} 560 nm (ε 16.2), 401 (ε 20.1), 310 (ε 218).

Gaswick, D. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 437 (*synth, uv-vis, isomer*)

$C_6H_{10}CoCrN_6O_5$ IC-005080

[Pentaaquachromium(*III*)]-μ-isocyano[pentacyanocobalt(*III*)]

Pentaaqua[μ-(cyano-N:C)][pentakis(cyano-C)cobalt]chromium

[67870-86-4]

$(H_2O)_5CrCNCo(CN)_5$

M 357.1

Made by rapid reaction of $[Co(CN)_5N_3]^{3\ominus}$ with nitrous acid in presence of $[Cr(OH_2)_5CN]^{2\oplus}$. Characterised in soln. λ_{max} 552 (ε 18.3), 347 (ε 231) nm.

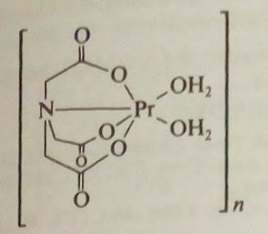
Gaswick, D. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 437 (*synth, uv-vis, isom*)

$C_6H_{10}NO_8Pr$ IC-005093

Diaqua(nitrilotriacetato)praseodymium(*III*)

Diaqua[N,N-bis(carboxymethyl)glycinato(3−)-N,O,O′,O″]praseodymium(III), 9CI. (Nitrilotriacetato)diaquopraseodymium(III)

[38893-89-9]



M 365.0

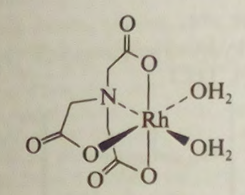
9-Coord. polymer with bridging nitriloacetato groups. Rectangular green prismatic cryst. + $1H_2O$.

Fitch, F.T. *et al, Can. J. Chem.*, 1951, **29**, 363 (*use*)
Mitrofanova, N.D. *et al, Zh. Neorg. Khim.*, 1962, **7**, 1049; 1964, **9**, 320; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 539; 1964, **9**, 174 (*synth*)
Martin, L.L. *et al, Inorg. Chem.*, 1972, **11**, 2785 (*cryst struct*)

$C_6H_{10}NO_8Rh$ IC-005094

Diaqua(nitrilotriacetato)rhodium(*III*), 8CI

[20658-37-1]



M 327.0

Octahedral. Pale yellow cryst.

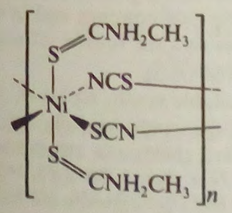
Smith, B.B., *Inorg. Chem.*, 1968, **7**, 922 (*synth, pmr*)

$C_6H_{10}N_4NiS_4$ IC-005095

Bis(ethanethioamide-*S*)bis(thiocyanato-*N*)nickel(*II*), 9CI

Bis(thioacetamide)bis(thiocyanato)nickel(II)

[21281-52-7]



M 325.1

Polymeric chain struct. with octahedral Ni and bridging NCS. Green cryst. μ_{eff} = 3.13μ_B (293K); Ir $\nu_{C\equiv N}$ 2118 cm^{-1}. Exhibits ferromagnetic coupling within chains, and antiferromagnetic coupling between chains.

[27071-29-0, 35232-22-5]

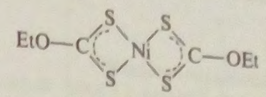
Nardelli, M. *et al, Gazz. Chim. Ital.*, 1958, **88**, 359 (*synth*)
Capacci, L. *et al, Acta Crystallogr., Sect. B*, 1968, **24**, 1199 (*cryst struct*)
Flint, C.D. *et al, J. Chem. Soc. A*, 1968, 750 (*synth, uv-vis, ir, magnetism*)
Emori, S. *et al, Bull. Chem. Soc. Jpn.*, 1971, **44**, 3299 (*magnetism*)

$C_6H_{10}NiO_2S_4$ IC-005096

Bis(*O*-ethyldithiocarbonto)nickel

Bis(O-ethylcarbonodithioato-S,S′)nickel, 9CI. Bis(hydrogen dithiocarbonato)nickel-O,O-diethylester, 8CI. Bis(ethylxanthato)nickel(II)

[21375-69-9]



M 301.0

Square planar; monomeric. Brown solid. Diamagnetic. Mp 136-138°.

[52139-56-7]

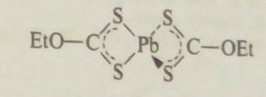
Watt, G.W. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 898 (*synth*)
Nanjo, M. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 2411 (*uv, ir, pmr*)
Hunt, M.R. *et al, Aust. J. Chem.*, 1971, **24**, 53, 161 (*ir*)
Mizota, T. *et al, CA*, 1981, **94**, 166005w (*cryst struct*)

$C_6H_{10}O_2PbS_4$ IC-005097

Bis(*O*-ethyl dithiocarbonato)lead(*II*)

Bis(ethylxanthato)lead. Bis(O-ethyl carbonodithioato-S,S)lead, 9CI. Lead(II) ethylxanthate

[23810-93-7]



M 449.6

Formed in the flotation of sulfide minerals by xanthates. Fine silvery needles (EtOH or Me_2CO). Mp 130°.

[5439-55-4]

Hagihara, H., *Acta Crystallogr.*, 1966, **21**, 350 (*cryst struct*)
Casey, A.T. *et al, Inorg. Chim. Acta*, 1987, **131**, 191 (*synth*)
Colthup, N.B. *et al, Spectrochim. Acta, Part A*, 1987, **43**, 317 (*ir*)

$C_6H_{10}O_2RuS_2$ IC-005098

Dicarbonylbis(ethanethiolato)ruthenium(*II*), 9CI

[32104-51-1]

$[Ru(CO)_2(SEt)_2]_n$

M 279.3

Polymeric or oligomeric compd., structures ranging from chains to clusters have been postulated. Prepd. by treating $Ru_3(CO)_{12}$ with EtSH or EtSSEt; forms where *n* has differing values are likely. Yellow-orange solid. Sol. CCl_4. Mp 59-60°. Ir ν_{CO} 2110, 2041, 1986 cm^{-1} (CCl_4).

[44970-88-9]

Johnson, B.F.G. *et al, Nature (London)*, 1967, **213**, 901 (*synth, ir*)
Cetini, G. *et al, J. Organomet. Chem.*, 1968, **15**, P4 (*synth, ir*)

$C_6H_{10}O_2S_4Zn$ IC-005099

Bis(*O*-ethyldithiocarbonato)zinc

Bis(O-ethyl carbonodithioato-S,S′)zinc. O,O-Diethyl bis(hydrogen dithiocarbonato)zinc. Zinc ethylxanthate. Bis(ethyl xanthato)zinc

[21757-57-3]

$(EtOCSS)_2Zn$

M 307.7

Polymeric struct. with tetrahedral Zn. Air-stable cryst. (EtOH). $Bp_{0.025-0.05}$ 120°. Forms complexes with pyridines, DMSO, phen.

Py complex: see *Bis(O-ethyl carbonodithioato-S,S′)(pyridine) zinc*, IC-007306
[13435-48-8]
Ikeda, T. *et al*, *Acta Crystallogr.*, 1966, **21**, 919 (*synth, cryst struct*)
Hunt, M.R. *et al*, *Aust. J. Chem.*, 1971, **24**, 53 (*ir, derivs*)
Cheremisina, I.M. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1971, **20**, 2032 (*ir*)

IC-005100

$C_6H_{10}O_2S_4Zn$

Bis(*O*-ethyldithiocarbonato)zinc
Bis(O-ethyl carbonodithioato-S,S′)zinc. Bis(hydrogen dithiocarbonato-O,O′)zinc diethyl ester. Bis(ethylxanthato) zinc. Zinc ethylxanthate
[13435-48-8]

$Zn(S_2COEt)$

M 307.7
Bridging xanthate groups; Zn tetrahedrally bound to 4 different xanthates in a 2D network. Cryst. Spar. sol. H_2O (1.35g per 100 cm^3); v. sol. EtOH; spar. sol. C_6H_6. Dec. at 140° (to β-ZnS).

[21757-57-3]
Ikeda, T. *et al*, *Acta Crystallogr.*, 1966, **21**, 919 (*synth, cryst struct*)
Hagashi, K. *et al*, *Bunseki Kagaku*, 1970, **19**, 325 (*stability const*)
Hunt, M.R. *et al*, *Aust. J. Chem.*, 1971, **24**, 53 (*ir*)
Shul'man, V.M. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **18**, 1587 (*synth, stability const*)
Raston, C.L. *et al*, *Aust. J. Chem.*, 1976, **29**, 731 (*uv*)

IC-005101

$C_6H_{10}O_4Sn$

Tin(*II*) propanoate
Bis(propanoato)tin. Tin(II) *propionate. Propanoic acid stannous salt*
[20004-09-5]

$Sn(OOCCH_2CH_3)_2$

M 264.8
White amorph. powder. Mp 140° (0.1 mm).

Donaldson, J.D. *et al*, *J. Chem. Soc. A*, 1968, 1448 (*mössbauer*)
Ewings, P.F.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1717 (*synth, ir, mössbauer*)

IC-005102

$C_6H_{10}O_4Zn$

Zinc(*II*) propanoate
Zinc propionate
[557-28-8]

$Zn(OOCCH_2CH_3)_2$

M 211.5
Propanoate groups bridge tetrahedral zinc → 2D polymeric struct. Wood preservative; antifungal agent; waterproofing agent; polym. catalyst. Thermal dec. to ZnO and $Zn_4O(OOCCH_2CH_3)_6$.

Monoclinic-form
Synth. from $ZnCO_3$ + propanoic acid in presence of propanoyl anhydride. Cryst.

Orthorhombic-form
Synth. from $Zn(OH)_2$ + aq. propanoic acid. Cryst.

[63745-19-7]
Goldschmied, E. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 2117 (*synth, cryst struct, monoclinic form*)
Panevchik, V.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1981, **26**, 1373; 1982, **27**, 1241 (*thermal anal, powder struct*)
Basei, P.S. *et al*, *Thermochim. Acta*, 1983, **71**, 15 (*thermal anal*)
Clegg, W. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 456 (*cryst struct, orthorhombic form*)

IC-005103

$C_6H_{10}O_6Pb$

Lead(*II*) lactate
Lead(II) *2-hydroxypropanoate. Bis(2-hydroxypropanoato-O¹,O²)lead*
[18917-82-3]

$Pb(OOCCHOHCH_3)_2$

M 385.3
White cryst. powder. Sol. cold H_2O, hot EtOH. Adsorbs CO_2 from air.
▷ Poisonous. OD5650000.

Basinski, A. *et al*, *Trans. Faraday Soc.*, 1965, **61**, 129 (*synth*)
Bottari, E. *et al*, *Gazz. Chim. Ital.*, 1971, **101**, 860; *CA*, **76**, 118079e (*formn*)
Kruhak, I. *et al*, *Croat. Chim. Acta*, 1976, **48**, 119 (*stab consts*)

IC-005104

$C_6H_{10}O_7Pb_2$

Lead(*II*) acetate hydroxide ($Pb_2(OAc)_3OH$)
Dilead hydroxide triacetate. Basic lead acetate ($Pb_2(OH)(OAc)_3$)

$Pb_2(OH)(OAc)_3$

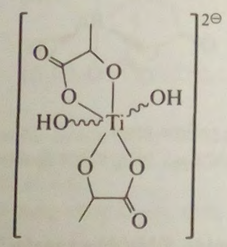
M 608.5
White solid. V. sol. H_2O; sl. sol. EtOH.

Grillot, E., *J. Chim. Phys. Phys.-Chim. Biol.*, 1946, **43**, 169; *CA*, 1947, **41**, 4396h.

IC-005105

$C_6H_{10}O_8Ti^{2\ominus}$

Dihydroxybis[2-hydroxypropanoato(2−)-*O*¹,*O*²]titanate(*IV*)(2−), 11CI



M 258.0 (ion)
Geometry unknown. Potential use as a binder of antibiotics to cotton, a primer for tinplate, as a cross-linking agent for pva coatings and in oil-well fluids, in jet-printing inks and the manuf. of molecular sieves.
Di-NH_4 salt: [65104-06-5].
No readily available synth. reported.

Japan. Pat., 58 134 164, (1983); *CA*, **100**, 122968a (*use*)
Japan. Pat., 58 78 517, (1983); *CA*, **100**, 8658z (*use*)
Morris, C.E. *et al*, *Text. Res. J.*, 1983, **53**, 143 (*use*)
Pat. Coop. Treaty (*WIPO*), 85 04 856, (1985); *CA*, **104**, 152267w (*use*)
U.S. Pat., 4 495 156, (1985); *CA*, **102**, 153132u (*use*)
U.S. Pat., 4 514 309, (1985); *CA*, **102**, 223193r (*use*)

IC-005106

$C_6H_{10}O_{10}Zn$

Diaquabis[propanedioato(1−)-*O*,*O*‴]zinc
Zinc bis(hydrogen malonate) dihydrate
[51378-86-0]

$Zn(OH_2)_2(OOCCH_2COOH)_2$

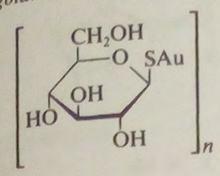
M 307.5
In solid state, Zn is octahedral (4 carboxylato O and 2 OH_2); $HO_2CCH_2CO_2^{\ominus}$ chains are cross-linked by Zn. Colourless prisms.

Waller-Levy, L. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 2596 (*synth, struct*)
Sinha, V.C. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1980, **152**, 157 (*cryst struct*)

IC-005107

$C_6H_{11}AuO_5S$

***C*-Thioglucopyranosato)gold, 9CI**
*(1-Thioglucopyranosato)gold. **Aurothioglucose***, INN, USAN



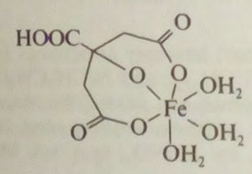
M 392.1
Polymeric.
p-form [12192-57-3]
Aureotan. Solganol. Aurumine. Oronol
Antiarthritic drug. Yellow cryst. (EtOH aq.). Sol. H_2O, insol. org. solvs.
▷ MD6475000.
Tetra-Ac: [69849-37-2]. *(1-Thioglucopyranosato-2,3,4,6-tetraacetato)gold, 10CI*
$C_{14}H_{19}AuO_9S$ M 560.3
Antiarthritic drug. Pale yellow cryst. (2-propanol/Et_2O). Mp 146-148°. $[\alpha]_D^{25}$ −56.9° (c, 1 in MeOH). Polymeric.

[74610-70-1, 82475-04-5]
Sadler, P.J., *Struct. Bonding* (*Berlin*), 1976, **29**, 171 (*rev*)
Lorber, A. *et al*, *Gold Bull.*, 1979, **12**, 149 (*rev*)
U.S. Pat., 4 133 952, (1979); *CA*, **90**, 152549g (*deriv*)
Brown, D.H. *et al*, *Chem. Soc. Rev.*, 1980, **9**, 217 (*rev*)
Brown, K. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4943 (*mössbauer*)
Shaw, C.F. *et al*, *J. Inorg. Biochem.*, 1981, **14**, 267 (*rev, cmr*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 5294.

IC-005108

$C_6H_{11}FeO_{10}$

Triaqua[citrato(3−)]iron
Ferric citrate trihydrate
[Hydrogencitrato(3−)]triaquoiron



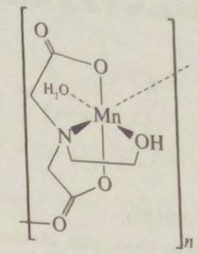
M 298.9
Compd. with choline: ***Ferrocholinate*, INN.** *Ferrocholine. Ferrochelate. Chelafer. Chel-Iron. Other synonyms*
$C_{11}H_{24}FeNO_{11}$ M 402.1
Haematinic. Brown amorph. powder.

U.S. Pat., 2 575 611; *CA*, **46**, 1722g (*synth, Ferrocholinate*)
Chakrabarti, J.K. *et al*, *Chem. Ind.* (*London*), 1961, 1407 (*synth, pharmacol, Ferrocholinate*)
Miller, E.R. *et al*, *J. Anim. Sci.*, 1981, **52**, 783 (*use*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 5042.

IC-005109

$C_6H_{11}MnNO_6$

Aqua(β-hydroxyethyliminodiacetato)manganese(*II*) monohydrate
Aqua[N-(*carboxymethyl*)(*2-hydroxyethyl*)*glycinato*(2−)] *manganese, 11CI*
[56404-98-9]



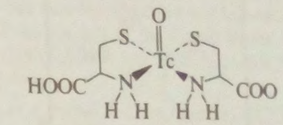
M 248.0
Polymeric chain struct. with one bridging carboxylate group. Pale pink cryst. + $1H_2O$.

Anan'eva, N.N. *et al*, *Koord. Khim.*, 1975, **6**, 850; 1981, **7**, 1556 (*synth, cryst struct*)

IC-005110

$C_6H_{11}N_2O_5S_2Tc$

Bis(cysteinato)oxotechnetium(*V*)



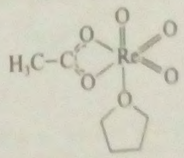
M 354.2
The Tc-cysteine system is not yet fully characterised; the Tc(*V*) complex probably has the struct. shown, perhaps with the $-CO_2^{\ominus}$ group interacting with the Tc as in Bis(3-mercaptovalinato)oxotechnetium(*V*), IC-007034. Similar complexes formed with cysteine ethyl ester, with acetylcysteine, and with ethyl cysteineate dimer. Synth. from $[TcO_4]^{\ominus}$ + cysteine using Sn(*II*) or excess of ligand as reductant, or by ligand exchange with $TcOCl_4^{\ominus}$ or $TcO(gluconate)_2$. Yellow complex, with maximum stability at pH 4. May be reduced to green Tc(*IV*) sp.

Subramanian, G. *et al*, *Eur. J. Nucl. Med.*, 1976, **1**, 243 (*synth, analogue*)
Zalutsky, M. *et al*, *Int. J. Nucl. Med. Biol.*, 1977, **4**, 53 (*synth, biodistribn*)
Steigman, J. *et al*, *J. Labelled Compd. Radiopharm.*, 1977, **13**, 162 (*synth, uv*)
Johannsen, B. *et al*, *J. Nucl. Med.*, 1978, **19**, 816 (*synth, electrochem, chromatog, partition coeff, analogues*)
Spies, H. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **447**, 215 (*formn kinetics, analogue*)

IC-005111

$C_6H_{11}O_6Re$

(Acetato-*O*,*O*′)trioxo(tetrahydrofuran)rhenium(*VII*), 11CI
(Acetato)trioxo(tetrahydrofuran)rhenium(VII)
[95419-28-6]



M 365.3

Synth. from Re_2O_7 and acetic anhydride in THF. Colourless, moisture-sensitive needles.

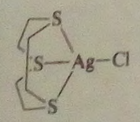
Edwards, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 2695 (*synth, ir, nmr, props*)

IC-005112

$C_6H_{12}AgClS_3$

Chloro(1,4,7-trithionane-S^1,S^4,S^7)silver(*I*)

[122539-96-2]



M 323.6

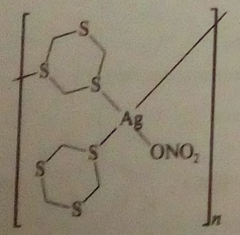
Colourless cryst. (MeOH).

Blower, P.J. *et al*, *Inorg. Chem.*, 1989, **28**, 4040 (*synth, cryst struct, ir*)

IC-005113

$C_6H_{12}AgS_6^{\oplus}$

Bis(*S*-trithiane)silver(1+)



Nitrate salt

M 384.4 (ion)

Nitrate: [24991-68-2]. *Silver(I) nitrate bis(1,3,5-trithiane)*

$C_6H_{12}AgNO_3S_6$ M 446.4

Large plates (hot H_2O). Dec. at 150°. Nitrate weakly coord. to Ag; polymeric chain struct.

Hexafluoroarsenate: [86529-69-3].

Cryst.

Domenicano, A. *et al*, *J. Chem. Soc. A*, 1968, 866 (*synth, cryst struct, nitrate*)

Hofman, H. *et al*, *J. Organomet. Chem.*, 1983, **249**, 97 (*synth, ir, cryst struct, hexafluoroarsenate*)

IC-005114

$C_6H_{12}AgSe_3^{\oplus}$

Bis(1,3,5-triselenane-Se^1,Se^3,Se^5)silver(*I*)(1+)

M 665.7 (ion)

Hexafluoroarsenate: [86526-38-7].

Yellow cryst. + $2SO_2$.

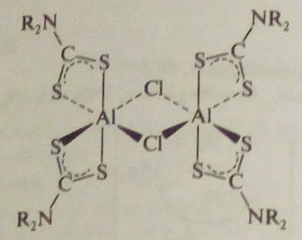
Hofman, H. *et al*, *J. Organomet. Chem.*, 1983, **249**, 97 (*synth, ir, cryst struct*)

$C_6H_{12}AlClN_2S_4$

IC-005115

Chlorobis(*N*,*N*'-dimethyldithiocarbamato)aluminium

Chlorobis(dimethylcarbamodithioato-S,S')aluminium



dimer

R = Me

M 302.8

Dimeric.

Dimer: [88118-23-4]. *Di-μ-chlorotetrakis(dimethylcarbamodithioato-S,S')dialuminium*

$C_{12}H_{24}Al_2Cl_2N_4S_8$ M 605.7

Synth. from $AlCl(NMe_2)_2$ + CS_2. Colourless moisture-sensitive cryst. Spar. sol. Et_2O, hexane; sol. C_6H_6, CH_2Cl_2, $CHCl_3$. Mp 150° dec.

Nöth, H. *et al*, *Chem. Ber.*, 1983, **116**, 3552 (*synth, ir, Al-27 nmr*)

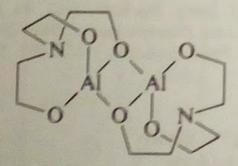
$C_6H_{12}AlNO_3$

IC-005116

[[2,2',2''-Nitrilotris[ethanolato]](3−)-*N*,*O*,*O*',*O*'']aluminium

Aluminium 2,2',2''-nitrilotriethoxide. 2,8,9-Trioxa-5-aza-1-aluminabicyclo[3.3.3]undecane

[21863-06-9]



dimer

M 173.1

Dimeric in vapour; hexamer or octamer in C_6H_6. Synth. from $Al[OCH(CH_3)_2]_3$ and $N(CH_2CH_2OH)_3$ in C_6H_6. Catalyst component in process for manuf. of propylene glycol. White moisture-sensitive cryst. (C_6H_6). Sol. $CHCl_3$, C_6H_6, Py, $MeNO_2$; spar. sol. Me_2CO. Mp 375° dec.

Dimer:

$C_{12}H_{24}Al_2N_2O_6$ M 346.2

Dioxan complex: Synth. from $Al(OCH_2CH_2)_3N$ + dioxan. Colourless cryst.

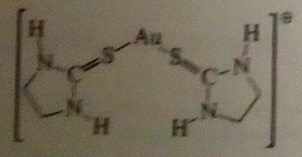
Hein, F. *et al*, *Z. Anorg. Allg. Chem.*, 1952, **269**, 67 (*synth, props*)
Mehrotra, R.C. *et al*, *J. Indian Chem. Soc.*, 1962, **39**, 677 (*synth*)
Lacey, M.J. *et al*, *Aust. J. Chem.*, 1976, **29**, 1119 (*ms*)

IC-005117

$C_6H_{12}AuN_4S_2^{\oplus}$

Bis(2-imidazolidinethione-*S*)gold(*I*)(1+), 10Cl

Bis(ethylenethiourea)gold(I)(1+)



M 401.2 (ion)

Chloride: [61593-59-7].

$C_6H_{12}AuClN_4S_2$ M 436.7

Cryst. + H_2O. Mp 210°, 242° dec. H_2O of crystallisation lost on heating to 110°. Geometry about Au not linear due to H-bonding to OH_2.

Morgan, G.T. *et al*, *J. Chem. Soc.*, 1928, 143 (*synth*)
Jones, P.G. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 3321 (*cryst struct*)
Jones, G.C.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1440 (*mössbauer*)

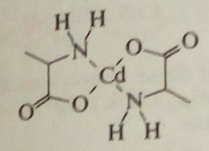
IC-005118

$C_6H_{12}CdN_2O_4$

Bis(alaninato-*N*,*O*)cadmium

Cadmium alaninate

[14221-39-7]



M 288.5

Prepd. from CdO + alanine. White cryst. Spar. sol. H_2O.

[15975-16-3, 28143-24-0, 85284-83-9]

Fedorov, A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1962, 7, 160 (*synth*)
Rao, G.N. *et al*, *Can. J. Chem.*, 1966, **44**, 1637 (*synth*)
Demaret, A. *et al*, *J. Appl. Crystallogr.*, 1983, **16**, 279 (*cryst struct*)

IC-005119

$C_6H_{12}CdN_2S_4$

Bis(*N*,*N*-dimethyldithiocarbamato)cadmium

Bis(dimethylcarbamodithioato-S,S')cadmium, 9CI

[14949-60-1]

$Cd(S_2CNMe_2)_2$

M 352.8

White solid. Mp >300°.

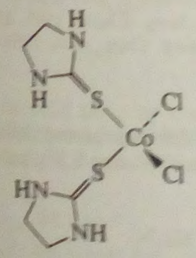
Geloso, G. *et al*, *Can. J. Chem.*, 1987, **65**, 928 (*electrochem synth*)
Frigerio, A. *et al*, *Inorg. Chim. Acta*, 1989, **164**, 149 (*synth, ir, raman*)

IC-005120

$C_6H_{12}Cl_2CoN_4S_2$

Dichlorobis(2-imidazolidinethione-*S*)cobalt(*II*)

Dichlorobis(ethylenethiourea)cobalt(II)



M 334.1

Probable tetrahedral struct. shown. Prepared from anhydrous $CoCl_2$ and ethylenethiourea in hot EtOH. Azure blue cryst. Sol. hot EtOH, Me_2CO. Paramagnetic.

Catlin, R.L., *Inorg. Chem.*, 1963, **2**, 849 (*synth, ir, props*)

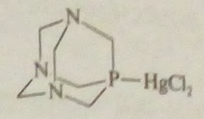
$C_6H_{12}Cl_2HgN_3P$

IC-005121

Dichloro(1,3,5-triaza-7-phosphatricyclo[3.3.1.1^{3,7}]decane-P^7)mercury, 12CI

Dichloro(1,3,5-triaza-7-phosphaadamantane)mercury. (1,3,5-Triaza-7-phosphaadamantane)mercury dichloride

[123073-14-3]



M 428.6

Prob. aggregated. Cryst. (MeOH). Insol. H_2O, org. solvs. Mp 213°.

Alyea, E.C. *et al*, *Can. J. Chem.*, 1989, **67**, 1319 (*synth, ir, raman, P-31 nmr*)

IC-005122

$C_6H_{12}Cl_2N_2O_2S_2Ti$

Dichlorobis(dimethylcarbamothioato-O,S)titanium(*IV*), 11CI

Dichlorobis(N,N-dimethylthiocarbamato)titanium(IV)

[86277-18-1]

$TiCl_2[SC(O)NMe_2]_2$

M 327.0

Octahedral but detailed structure not known. Synth. from $TiCl_4$ and the Na salt of the ligand under reflux in CH_2Cl_2. Orange solid. Sol. $CHCl_3$; sl. sol. C_6H_6. Mp 150-152° dec.

Gupta, V.D. *et al*, *Indian J. Chem., Sect. A*, 1983, **22**, 250 (*synth, ir, pmr*)

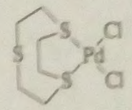
IC-005123

$C_6H_{12}Cl_2PdS_3$

cis-Dichloro(1,4,7-trithionane-S^1,S^4)palladium(*II*), 12CI

Dichloro(1,4,7-trithiacyclononane)palladium(II)

[109994-16-3]



M 357.6

cis-Square planar at Pd. Dark red cryst. ($MeNO_2$). Corresp. bromide is isostructural.

Blake, A.J. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 360 (*synth, cryst struct*)

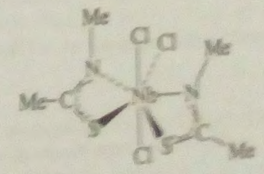
IC-005124

$C_6H_{12}Cl_3N_2NbS_2$

Trichlorobis(*N*-methylthioacetamido)niobium(*V*)

Trichlorobis(N-methylethanethioamidato-N,S)niobium(V), 9CI

[51975-95-2]



M 375.5

Synth. from MeNCS + Me_2NbCl_3 in pentane. Example of the insertion of MeNCS into a Nb—C bond. Dark red cryst.

Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 198 (*cryst struct*)
Wilkins, J.D., *J. Organomet. Chem.*, 1974, **65**, 383 (*synth, ir, pmr*)

$C_6H_{12}Cl_3N_3O_6Ti^{3\ominus}$ IC-005125

Trichlorotris(glycinato-*N*)titanate(*III*)(3−), 11CI

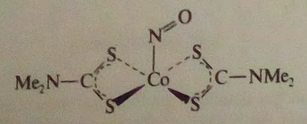
$[(OOCCH_2NH_2)_3TiCl_3]^{3\ominus}$

M 376.4 (ion)
Octahedral coord. at Ti.
Tri-H compd.: [91731-29-2]. *Trichlorotris(glycine-N)titanium*(III)
$C_6H_{15}Cl_3N_3O_6Ti$ M 379.4
Synth. by mixing 1 mol $TiCl_3$ in HCl and 3 mol aq. glycine. Grey solid.

Castillo, M. *et al*, *Transition Met. Chem.*, 1984, **9**, 268 (*synth, ir*)

$C_6H_{12}CoN_3OS_4$ IC-005126

Bis(*N,N*-dimethyldithiocarbamato)nitrosylcobalt(*I*)
Bis(dimethylcarbamodithioato-S,S′)nitrosylcobalt, 9CI
[36434-42-1]

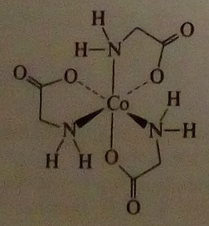


M 329.3
Bent nitrosyl coordination, square pyramidal at Co. Black-brown cryst.

Enemark, J.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 718 (*synth, cryst struct*)
Ileperuma, O.A. *et al*, *Inorg. Chem.*, 1976, **16**, 7 (*synth*)

$C_6H_{12}CoN_3O_6$ IC-005127

Tris(glycinato-*N,O*)cobalt(*III*), 11CI
[14221-43-3]



fac-form

M 281.1
Variations in synthetic procedure afford different mixtures of isomers. Once formed, isomers are not readily interconverted. Coordinated glycine activated - condenses with acetaldehyde to yield threonine. Metabolised selectively by a bacterium.

fac-form
β-form
Red-pink needles; also reported as $+1H_2O$. V. sol. H_2O.

mer-form
α-form
More stable isomer. Dark violet cryst. $+ 1H_2O$; also reported as $+ 2H_2O$. Has been resolved.

[21520-57-0, 27074-68-6, 30364-77-3, 55658-12-3, 79466-46-9, 79516-75-9]

Ley, H. *et al*, *Ber.*, 1909, **42**, 3894 (*synth, mer-form*)
Krebs, H. *et al*, *Z. Anorg. Allg. Chem.*, 1954, **276**, 236 (*resoln*)

Neville, R.G. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 4895 (*synth, fac-form*)
Ikutani, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1959, **32**, 203 (*reaction*)
Mori, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1961, **34**, 1837 (*synth, mixed forms*)
Gillard, R.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 997 (*metabolism, cd*)
Norman, P.R. *et al*, *Inorg. Chim. Acta*, 1977, **24**, L35 (*reactions*)
Dewan, J.C., *Acta Crystallogr., Sect. C*, 1988, **44**, 2199 (*cryst struct*)
Inorg. Synth., 1989, **25**, 135 (*synth, bibl*)

$C_6H_{12}CrN_2S_4$ IC-005128

Bis(*N,N*-dimethyldithiocarbamato)chromium(*II*)
Bis(dimethylcarbamodithioato-S,S′)chromium(II), *11CI*
Chromium(II) *dimethyldithiocarbamate*
[104050-56-8]

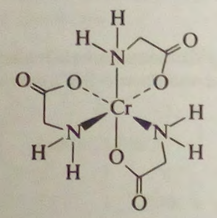
$Cr(S_2CNMe_2)_2$

M 292.4
Possibly *S*-bridged dimer or polymer. Red, air-sensitive solid. μ_{eff} = 4.45μ_B (300K), 4.07μ_B (90K). Antiferromagnetic.

Larkworthy, L.F. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 139.
Tanaka, M. *et al*, *Polyhedron*, 1986, **5**, 703.

$C_6H_{12}CrN_3O_6$ IC-005129

Tris(glycinato-*N,O*)chromium(*III*), 11CI, 10CI
Chromium(III) *glycinate*
[14320-13-9]



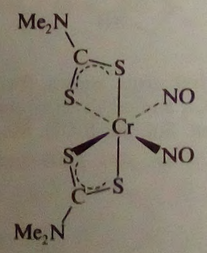
M 274.1
fac-Octahedral molecule. Crimson cryst. + H_2O. Spar. sol. H_2O; insol. org. solvs.

[14325-26-9, 30596-51-1]

Bryan, R.F. *et al*, *Inorg. Chem.*, 1971, **10**, 1468 (*cryst struct, synth, uv-vis*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1519 (*synth*)
Wallace, W.M. *et al*, *Inorg. Chem.*, 1983, **22**, 491 (*photochem*)
Cooper, J.A. *et al*, *Inorg. Chim. Acta*, 1984, **92**, 23 (*synth*)

$C_6H_{12}CrN_4O_2S_4$ IC-005130

Bis(*N,N′*-dimethyldithiocarbamato)dinitrosylchromium
Bis(dimethylcarbamodithioato-S,S′)dinitrosylchromium, 11CI
[87458-65-9]



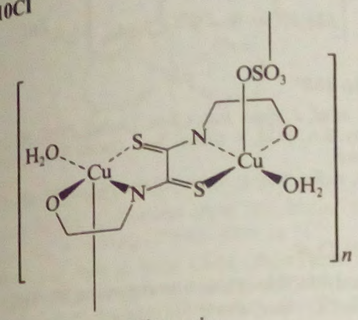
M 352.4

Example of a dinitrosylchromium complex. *cis*-Octahedal. Purple red cryst. (MeOH). Sol. org. solvs. Mp 215° dec. Ir ν_{NO} 1805, 1684 cm^{-1}. Diamagnetic.

Carlin, R.L. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 898 (*synth*)
Herberhold, M. *et al*, *Chem. Ber.*, 1983, **116**, 2896 (*synth, ir, nmr*)

$C_6H_{12}Cu_2N_2O_4S_2^{2\oplus}$ IC-005131

Diaqua[*N,N′*-bis(2-hydroxyethyl)ethanedithioamidato(2−)-*N,O,S*:*N′,O′,S*]dicopper(*II*)(2+), 10CI



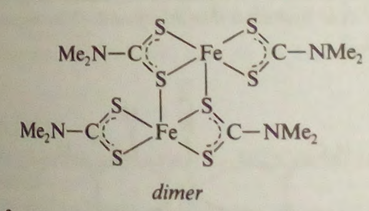
Sulfate salt

M 367.3 (ion)
Cu—Cu 561 pm.
Sulfate: [67408-44-0]. catena-*μ-Sulfato*-[N,N′-*bis*(2-*hydroxyethyl*)*dithiooxamido*(2−)-N,O,S:N′,O′,S′]*bis*[*aquacopper*(II)]
Dark green sl. air sensitive cubic cryst. (conc. H_2SO_4). Insol. H_2O. Dimeric units are linked into chain struct. via sulfate anions.

Girerd, J.J. *et al*, *Inorg. Chem.*, 1978, **17**, 3034 (*synth, cryst struct, magnetism*)
Kahn, O., *Inorg. Chim. Acta*, 1982, **62**, 3 (*rev*)

$C_6H_{12}FeN_2S_4$ IC-005132

Bis(*N,N*-dimethyldithiocarbamato)iron(*II*)
Bis(dimethylcarbamodithioato-S,S′)iron(II), *9CI*
[15339-38-5]



dimer

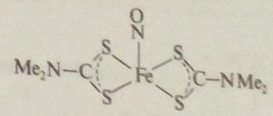
M 296.2
Probably dimeric in solid state by analogy with Bis(*N,N*-diethyldithiocarbamato)iron(*II*), IC-007065. Catalyst, biocide, photocatalyst, antifouling agent.

Dimer:
$C_{12}H_{24}Fe_2N_4S_8$ M 520.5

Pignolet, L.H. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 360 (*synth*)
de Vries, J.L.K. *et al*, *Inorg. Chem.*, 1973, **12**, 2730 (*synth, mössbauer, magnetism*)

$C_6H_{12}FeN_3OS_4$ IC-005133

Bis(dimethyldithiocarbamodithioato-*S,S′*)nitrosyliron, 9CI
Bis(dimethyldithiocarbamato)nitrosyliron, 8CI
[14263-11-7]

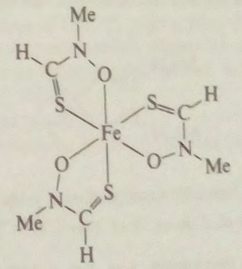


M 326.2
Square pyramidal complex; angle: FeNO 170°. Synth. from $FeSO_4.7H_2O$ in H_2O; soln. satd. with NO followed by addn. of NaS_2CNMe_2. Stable dark-green cryst. giving yellow-green solns. Sol. $CHCl_3$, CS_2, C_6H_6. Paramagnetic. Characterised by: Ir ν_{NO} 1690 cm^{-1} (KBr); ν_{NO} 1724 cm^{-1} ($CHCl_3$).

Cambi, L. *et al*, *CA*, 1932, **26**, 41 (*synth*)
Gray, H.B. *et al*, *J. Am. Chem. Soc.*, 1962, **84**, 3404 (*uv, esr*)
Gibson, J.F., *Nature (London)*, 1962, **196**, 62 (*esr*)
Danon, J., *J. Chem. Phys.*, 1964, **41**, 3378 (*mössbauer*)
McNeil, D.A.C. *et al*, *Proc. Chem. Soc., London*, 1964, 364 (*esr*)
Colapietro, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 583 (*analogue, struct*)
Johnson, C.E. *et al*, *J. Chem. Phys.*, 1969, **50**, 2594 (*mössbauer*)
Davies, G.R. *et al*, *J. Chem. Soc. A*, 1970, 1275 (*struct*)
Miki, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **96**, 3779 (*ir*)
Enemark, J.H. *et al*, *Coord. Chem. Rev.*, 1974, **13**, 363 (*rev*)
Ileperuma, O.A. *et al*, *Inorg. Chem.*, 1977, **16**, 1876 (*synth*)
Quinby-Hunt, M. *et al*, *Inorg. Chem.*, 1978, **17**, 2515 (*ir*)
Sarte, B. *et al*, *Inorg. Chem.*, 1978, **17**, 3361 (*ir, esr, mössbauer, analogues*)
Fitzsimmons, B.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1548 (*mössbauer*)
Feltman, R.D. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 37 (*esr*)
Ganguli, P. *et al*, *J. Phys. Colloq.*, 1980, 317 (*electronic struct*)
Butler, A.R. *et al*, *Polyhedron*, 1985, **4**, 797 (*esr, analogues*)

$C_6H_{12}FeN_3O_3S_3$ IC-005134

Fluopsin B
Tris(N-*hydroxy*-N-*methylmethanethioamidato*-O,S)*iron, 9CI*
Fluopsin F
[31323-26-9]



M 326.2
Isol. from *Pseudomonas fluorescens*. Broad spectrum antibiotic with antifungal and antineoplastic props. Black prisms ($MeOH/CHCl_3$). Dec. on heating.

▷ NO8780000.

Shirahata, K. *et al*, *J. Antibiot.*, 1970, **23**, 546 (*isol, struct*)
Mitchell, A.J. *et al*, *Aust. J. Chem.*, 1977, **30**, 2439 (*synth*)
Murray, K.S. *et al*, *Aust. J. Chem.*, 1978, **31**, 983 (*cryst struct*)
Leong, J. *et al*, *Inorg. Chem.*, 1978, **17**, 1886 (*ir, nmr, synth*)
Bell, S.J. *et al*, *Antimicrob. Agents Chemother.*, 1979, **15**, 384 (*props*)

IC-005135

$C_6H_{12}HgN_2O_4S_2$
Bis(cysteinato)mercury
[12550-82-2]

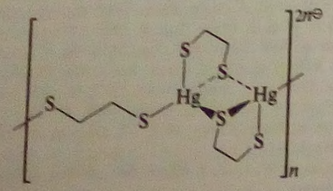
$[HSCH_2CH(NH_2)COO]_2Hg$

M 440.8
Mono-HCl: [52700-45-5].
Prepd. from $HgCl_2$ + L-cysteine-HCl. White cryst. + $\frac{1}{2}H_2O$.
Di-Me ester, di-HCl: [21496-19-5].
Prepd. from $HgCl_2$ + L-cysteine methyl ester hydrochloride. White cryst. + $1H_2O$. Sol. H_2O.
[14724-38-0, 108032-83-3]

Shindo, H. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 1904 (*ir*)
Hay, R.W. *et al*, *Aust. J. Chem.*, 1967, **20**, 675 (*synth, ir, Me ester*)
Neville, G.A. *et al*, *Can. J. Chem.*, 1973, **51**, 3970; 1974, **52**, 616 (*synth, cmr*)
Sze, Y.K. *et al*, *Inorg. Chem.*, 1975, **14**, 1969 (*ir, raman*)

IC-005136

$C_6H_{12}Hg_2S_6^{2\ominus}$
Bis[μ-[1,2-ethanedithiolato(2−)-*S:S,S'*]][1,2-ethanedithiolato(2−)-*S,S'*]dimercurate(2−)

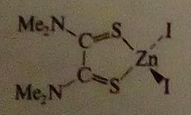


M 677.7 (ion)
Polymeric anion.
Bis-Ph_4P salt: [101461-93-2].
Cryst. (MeOH).

Henkel, G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 1498 (*synth, cryst struct*)

IC-005137

$C_6H_{12}I_2N_2S_2Zn$
Diiodo(tetramethylethanedithioamide-*S,S'*)zinc, 9CI
Zinc(II) *iodide tetramethylethanedithioamide*
[54184-39-3]

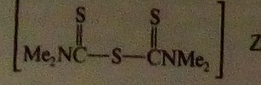


M 495.5
White solid. Cl and Br analogues also prepd.

Fabretti, A.C. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 1751 (*synth, ir*)
Geboes, P. *et al*, *Spectrochim. Acta, Part A*, 1988, **44**, 963 (*synth, ir*)

IC-005138

$C_6H_{12}I_2N_2S_3Zn$
Diiodo(tetramethyltrithiodicarbonic diamide)zinc
Zinc(II) *iodide* (*tetramethyltrithiodicarbonic diamide*)
[55913-70-7]



M 527.5
Yellow cryst. Insol. Et_2O.

McCleverty, J.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2169 (*synth, ir, pmr*)

IC-005139

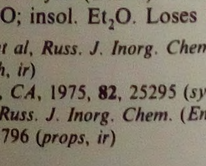
$C_6H_{12}I_2N_2S_4Zn$
Diiodo(tetramethylthiuram disulfide)zinc
Diiodo(*tetramethyl tetrathioperoxydicarbonic diamide*)*zinc*
[56031-14-2]

M 559.6
Cryst. Mp 165°.

Prasad, S. *et al*, *J. Proc. Inst. Chem.* (*India*), 1958, **30**, 259 (*synth*)
McCleverty, J.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2169 (*reactions*)
Srivastava, A.K. *et al*, *J. Indian Chem. Soc.*, 1983, **60**, 490 (*synth, ir*)

IC-005140

$C_6H_{12}MnN_2O_2S_2$
Bis(ethanol)bis(thiocyanato)manganese(*II*), 10CI
Manganese(II) *thiocyanate bis*(*ethanol*)
[25280-32-4]

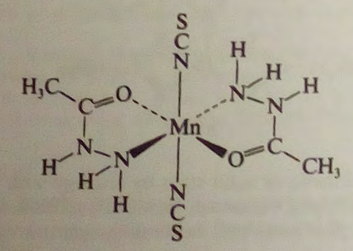


M 263.2
Struct. comprises polymeric sheets of thiocyanate bridged $Mn^{2\oplus}$ ions. Moisture-sensitive, pale green prisms (EtOH); loses EtOH in a dry atm.

McElearney, J.N. *et al*, *Phys. Rev. B*, 1979, **19**, 306 (*synth, cryst struct*)

IC-005141

$C_6H_{12}MnN_6O_2S_2$
Bis(acetylhydrazine-*N,O*)diisothiocyanatomanganese(*II*)
Bis(*acetic acid hydrazide*)*bis*(*thiocyanato*-N)*manganese*, *9CI*
[56603-57-7]



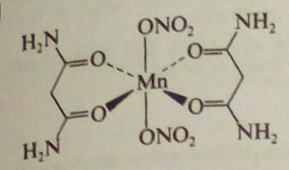
M 319.2
Hemihydrate: [52594-66-8].
Synth. from aq. solns. of $Mn(NCS)_2$ and $CH_3CONHNH_2$. Air-stable sky blue cryst. (H_2O). Distorted octahedral complex. H_2O forms H-bonds.
Monohydrate: Synth. from $Mn(NCS)_2$ and $CH_3CONHNH_2$ in EtOH. Sky blue cryst. (EtOH). V. sol. H_2O, EtOH; sol. DMF, DMSO; insol. Et_2O. Loses H_2O at 110°.

Kharitonov, Yu.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 613 (*synth, ir*)
Tsintsadze, G.V. *et al*, *CA*, 1975, **82**, 25295 (*synth*)
Kharitonov, Yu.Ya., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 540; 1977, **22**, 1796 (*props, ir*)

Tsintsadze, G.V. *et al*, *Soobshch. Akad. Nauk. Gruz. SSR*, 1984, **115**, 537; *CA*, 1985, **102**, 123483 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 169 (*rev, bibl*)

IC-005142

$C_6H_{12}MnN_6O_{10}$
Bis(nitrato-*O*)bis(propanediamide-*O,O'*)manganese(*II*), 10CI
Bis(*diamidomalonate*)*dinitratomanganese*
[74277-93-3]



M 383.1
Synth. from $Mn(NO_3)_2$ and $H_2NCOCH_2CONH_2$ in refluxing EtOH. Colourless cryst. Sol. H_2O, DMF, DMSO. $\mu_{eff} = 6.01\mu_B$ (298K). Dec. at 215°.

Tsivadze, A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 556, 866 (*synth, ir, raman*)
Aggarwal, R.C. *et al*, *Indian J. Chem., Sect. A*, 1980, **19**, 137 (*synth, props*)
Porai-Koshits, M.A. *et al*, *Koord. Khim.*, 1980, **6**, 793; *CA*, **93**, 58745 (*cryst struct*)
Smirnov, A.N. *et al*, *Sov. J. Coord. Chem.* (*Engl. Transl.*), 1980, **6**, 831 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 122 (*rev, bibl*)

IC-005143

$C_6H_{12}MnO_5$
Aquabis(propanoato-*O*)manganese(*II*), 10CI
[64337-86-6]

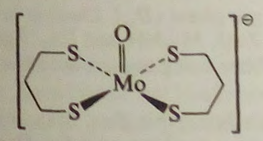
$[Mn(OOCCH_2CH_3)_2(OH_2)]_n$

M 219.0
Octahedral Mn in polymeric struct. Synth. from stoichiometric amounts of $Mn(OH)_2$ and H_3CCH_2COOH. Cryst. + $1H_2O$. $\mu_{eff} = 5.9\mu_B$ (78-295K).

Lis, T., *Acta Crystallogr., Sect. B*, 1977, **33**, 2964 (*synth, cryst struct, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 66 (*rev, bibl*)

IC-005144

$C_6H_{12}MoOS_4^{\ominus}$
Oxobis[1,3-propanedithiolato(2−)-*S,S'*]molybdate(*V*) (1−), 11CI
Bis(*propane-1,3-dithiolato*-S,S')*oxomolybdate*(V)(*1−*)

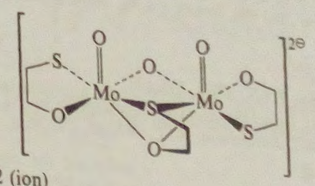


M 324.3 (ion)
Tetragonal pyramidal at Mo.
Ph_4P salt: [84534-63-4].
Dark blue-green cryst.

Bishop, P.T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 1052 (*cryst struct, synth*)

IC-005145

$C_6H_{12}Mo_2O_6S_3^{2\ominus}$
μ-Oxo-μ-2-mercaptoethanolatobis[oxo(2-mercaptoethanolato)molybdate(*V*)](2−)
[μ-[2-*Mercaptoethanolato*(2−)-O,S:O,S]]*bis*[2-*mercaptoethanolato*(2−)-O,S]-μ-*oxodioxodimolybdate*(V)(2−), *10CI*

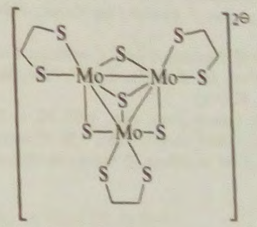


M 468.2 (ion)
Square pyramidal geometry about Mo atoms, with additional distant coordination to O in $^{\ominus}OCH_2CH_2S^{\ominus}$ bridge. Interatomic distances; Mo—Mo 267.6, Mo=O 170.0, 169.8 pm.
Bis-piperidinium salt: [71382-10-0].
Red cryst. (hot MeOH or hot Py). Sol. H_2O, MeOH; spar. sol. piperidine, higher alcohols. $\mu_{eff} = 0.12\mu_B$ (291K).

Dance, I.G. *et al*, *Inorg. Chem.*, 1979, **18**, 3487 (*cryst struct, synth, ir, uv-vis, magnetism*)

IC-005146

$C_6H_{12}Mo_3S_{10}^{2\ominus}$
μ_3-Sulfidotri-μ_2-sulfidotris(1,2-ethanedithiolato)trimolybdate(*IV*)(2−)
Tris[*1,2-ethanedithiolato*(2−)-S,S']*tri-μ-thioxo-*μ_3-*thioxotrimolybdate*(IV)(2−), *11CI*

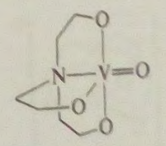


M 692.6 (ion)
Equilateral triangle of Mo(*IV*) atoms; Mo—Mo 277-279 pm. Resonance raman spectra suggest an analogy with the Fe_3S_4 core in some metalloproteins. Ir *v* 490, 475, 455, 355 cm^{-1} (KBr).
Bis-Et_4N salt: [88765-89-3].
Mod. air-stable violet black cryst. (MeCN/2-propanol). Sol. MeCN.

Halbert, T.R. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 1849 (*cryst struct, synth, ir, raman*)

IC-005147

$C_6H_{12}NO_4V$
[[2,2',2''-Nitrilotris[ethanolato]](3−)-*N,O,O',O''*]oxovanadium(*V*), 11CI
[(2,2',2''-*Nitrilotriethanolato*)(3−)]*oxovanadium*(V), *8CI*
Oxo[*triethanolaminato*(3−)]*vanadium*(V)
[15364-25-7]



M 213.1

Synth. from ethyl ortho-vanadate and triethanolamine in C_6H_6. Catalyses the rearrangement of unsatd. alcohols eg. dehydrolinalol to citral. Yellow solid.

[16698-96-7]

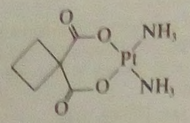
Mittal, R.K., *Z. Anorg. Allg. Chem.*, 1967, **351**, 309 (*synth*)
Chabardes, P. *et al*, *Tetrahedron*, 1977, **33**, 1775 (*synth, use*)
U.S.S.R. Pat., 882 998, (1981); *CA*, **96**, 162983g (*use*)

$C_6H_{12}N_2O_4Pt$ IC-005148

Carboplatin, BAN, INN, USAN

Diammine[1,1-cyclobutanedicarboxylato(2−)-O,O′]-platinum, 9CI. Paraplatin. NSC 241240. CBDCA. JM 8

[41575-94-4]



M 371.2

Antineoplastic drug. White solid. Sol. H_2O.

▷ TP2300000.

Ger. Pat., 2 329 485, (1973); *CA*, **81**, 21172v (*synth, pharmacol*)
Cleare, M.J. *et al*, *Platinum Met. Rev.*, 1973, **17**, 2 (*pharmacol*)
Harrison, R.C. *et al*, *Inorg. Chim. Acta*, 1980, **46**, L15 (*synth*)
Neidle, S. *et al*, *J. Inorg. Biochem.*, 1980, **13**, 205 (*cryst struct, pmr, cmr, Pt-195 nmr*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 16564.
Hopkins, S.J., *Drugs of the Future*, 1983, **8**, 489 (*rev*)
Al-Takhin, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2657 (*enthalpy of formation*)
Lelieveld, P. *et al*, *Eur. J. Cancer Clin. Oncol.*, 1984, **20**, 1087 (*props*)
Hacker, M.P. *et al*, *Platinum Coord. Complexes Cancer Chemother., Proc. Int. Dev. Oncol., v17, 1984*, Martinus Nijhoff, Boston, 1984, 82 (*rev*)
Rose, W.C. *et al*, *Cancer Treat. Rep.*, 1985, **12**, 1, 21, 145.
Beagley, B. *et al*, *J. Mol. Struct.*, 1985, **130**, 97 (*cryst struct*)
Zee-Cheng, R.K.Y. *et al*, *Drugs of Today (Barcelona)*, 1987, **23**, 563 (*rev*)

$C_4H_{12}N_2O_4S_2Zn$ IC-005149

Bis(L-cysteinato)zinc

[111231-27-7]

$[HSCH_2C(NH_2)HCOO]_2Zn$

M 305.6

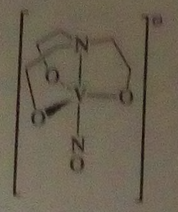
[73479-67-1]

Perrin, D.D. *et al*, *J. Chem. Soc. A*, 1968, 53 (*stability const*)
Sato, A. *et al*, *CA*, 1985, **103**, 47278 (*synth*)
Cole, A. *et al*, *Inorg. Chim. Acta*, 1985, **108**, 165 (*stability const*)
Kravchenko, V.S. *et al*, *CA*, 1988, **108**, 11509 (*ir*)

$C_6H_{12}N_2O_4V^{\ominus}$ IC-005150

[[2,2′,2″-Nitrilotris[ethanolato]](3−)-*N,O,O′,O″*]nitrosylvanadate(1−), 1CI

Nitrosyl[triethanolaminato(3−)]vanadate(1−). (2,2′,2″-Nitrilotriethoxy)nitrosylvanadate(1)(1−)



M 227.1 (ion)

Trigonal bipyramidal with linear VNO grouping. See also Cyano(2,2′,2″-nitrilotriethoxy)nitrosylvanadate(*1*)(2−), IC-005757.

Na salt, $NaClO_4$ complex (1:1): [101754-17-0].

Synth. by adding $NaClO_4$ to an alkaline soln. of NH_4VO_3, triethanolamine and hydroxylamine, extracting with C_6H_6. Red cryst. + $4H_2O$ (alkaline H_2O). Sol. H_2O. Acidic aq. solns. under Ar change from red to yellow. Ir ν_{NO} 1490 cm^{-1}. Interatomic distance: N—O 125.4 pm.

▷ Potentially explosive.

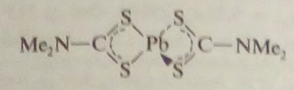
Wieghardt, K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 2493 (*synth, cryst struct, ir, uv-vis*)

$C_6H_{12}N_2PbS_4$ IC-005151

Bis(*N,N*-dimethyldithiocarbamato)lead(*II*)

Bis(dimethylcarbamodithioato-S,S′)lead, 9CI

[19010-66-3]



M 447.6

Synth. from $Pb(OAc)_2$ + Me_2NCS_2K. Used for curing rubber. Pale yellow needles (Me_2CO). Mp 258°.

▷ OF8850000.

[109707-89-3]

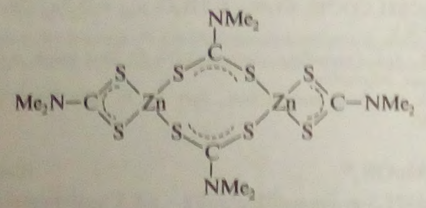
Jensen, K.A. *et al*, *Acta Chem. Scand.*, 1971, **25**, 2029 (*synth, ir*)
Iwasaki, H., *Acta Crystallogr., Sect. B*, 1980, **36**, 2138 (*cryst struct*)
Casey, A.T. *et al*, *Inorg. Chim. Acta*, 1987, **131**, 191 (*synth*)

$C_6H_{12}N_2S_4Zn$ IC-005152

Bis(*N,N*-dimethyldithiocarbamato)zinc, 8CI

Bis(dimethylcarbamodithioato-S,S′)zinc, 9CI. Ziram, BSI. Zirame. Milbam. Zerlate. Fuklasin

[137-30-4]



Dimer

M 305.8

Monomeric in gas phase (D_{2d}). Dimeric in solid state. Synth. from ZnO, Me_2NH and CS_2. Agricultural fungicide; rubber vulcanisation accelerator. Dec. by $H^{\oplus}$, uv light.

▷ Irritant. Forms inflammable dust. May be carcinogenic and mutagenic. Incompatible with Cu, Hg salts. ZH0525000.

Dimer: Bis[μ-(dimethylcarbamodithioato-S:S′)]bis(dimethylcarbamodithioato-S,S′)dizinc

$C_{12}H_{24}N_4S_8Zn_2$ M 611.6

Pale yellow cryst. ($CHCl_3$ or $CHCl_3$/EtOH). Insol. H_2O; spar sol. org. solvs. Mp 257° (250°).

Py complex (monomeric): [14642-29-6]. *Bis*(N,N-dimethyldithiocarbamato)*pyridine zinc*

$C_{11}H_{17}N_3S_4Zn$ M 384.9

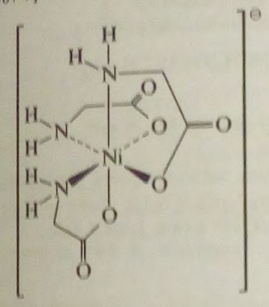
Vulcanisation catalyst. Needles + ½ C_6H_6 (C_6H_6). Insol. pet. ether. Sinters at 225°. Dissoc. in soln. with loss of Py.

Higgins, G.M.C. *et al*, *J. Chem. Soc.*, 1963, 2812 (*Py complex, synth*)
Klug, H.P., *Acta Crystallogr.*, 1966, **21**, 536 (*cryst struct*)
Fraser, K.A. *et al*, *Acta Crystallogr.*, 1967, **22**, 75 (*Py complex, cryst struct*)
Benson, W.R. *et al*, *J. Assoc. Off. Anal. Chem.*, 1968, **51**, 347 (*ms*)
Pilipenko, A.T. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 236 (*synth, ir*)
Coleman, M.M. *et al*, *Rubber Chem. Technol.*, 1973, **46**, 938 (*raman*)
Onuska, F.I. *et al*, *J. Assoc. Off. Anal. Chem.*, 1976, **59**, 622 (*ms*)
Tewari, S.N. *et al*, *J. Chromatogr.*, 1979, **172**, 528 (*tlc*)
Oktaec, D. *et al*, *Collect. Czech. Chem. Commun.*, 1980, **45**, 1495 (*ir*)
McCleverty, J.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1939 (*pmr, ir*)
Gustafsson, K.H. *et al*, *J. Agric. Food Chem.*, 1983, **21**, 461 (*hplc*)
Casey, A.T. *et al*, *Transition Met. Chem.*, 1986, **11**, 366 (*synth*)
Geloso, C. *et al*, *Can. J. Chem.*, 1987, **65**, 928 (*electrosynth*)
Pesticide Manual, 8th Ed., 1987, No. 12420.
Piegorsch, W.W. *et al*, *Mutat. Res.*, 1988, **196**, 161 (*haz*)
Hagen, K. *et al*, *Inorg. Chem.*, 1989, **28**, 3239 (*synth, ed*)
Merck Index, 11th Ed., 1989, No. 10075.

$C_6H_{12}N_3NiO_6^{\ominus}$ IC-005153

Tris(glycinato)nickelate(*II*)(1−), 8CI

[14362-87-9]



fac-form

M 280.8 (ion)

Component of lithographic desensitizing solns.

fac-form

More stable isomer.

K salt: [29636-22-4].

$C_6H_{12}KN_3NiO_6$ M 319.9

Blue solid.

Na salt, $NaClO_4$ adduct: [78919-05-8].

$C_6H_{12}ClN_3Na_2NiO_{10}$ M 426.2

Blue cryst. + D_2O.

mer(?)-form

Na salt:

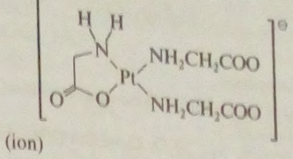
$C_6H_{12}N_3NaNiO_6$ M 303.8

Green cryst. Stereochem. not confirmed.

Hidaka, J. *et al*, *Bull. Chem. Soc. Jpn.*, 1970, **43**, 2999 (*synth, uv, cd*)
Pont, L.O. *et al*, *Inorg. Chem.*, 1974, **13**, 483 (*pe*)
Campana, C.F. *et al*, *Inorg. Chem.*, 1981, **20**, 4039.

$C_6H_{12}N_3O_6Pt^{\ominus}$ IC-005154

Tris(glycinato)platinate(*II*)(1−), 8CI



M 417.2 (ion)

Unusual example of mixed mono- and bidentate glycinate. Early report describes impossible isomerism.

K salt: [21791-03-7].

Props. not described.

Ag salt: [68736-54-9].

White solid + $2H_2O$.

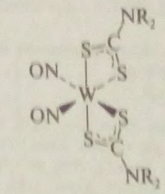
Grinberg, A.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1935, **2**, 485 (*synth*)
Volshtein, L.I. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1960, **5**, 840 (*synth*)
Erickson, L.E. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 6371 (*pmr*)
Astakhova, N.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 1513 (*ir, dta*)

$C_6H_{12}N_4O_2S_4W$ IC-005155

Bis(*N,N*-dimethyldithiocarbamato)dinitrosyltungsten

Bis(dimethylcarbamodithioato-S,S′)dinitrosyltungsten, 11CI, 10CI

[67180-13-6]



R = Me

M 484.3

Monomeric, octahedral complex.

cis-form

Synth. from Dibromodinitrosyltungsten, IC-001846 and excess sodium dimethyldithiocarbamate. Green needles (MeOH). Sol. org. solvs. Mp ⩾ 300°. $Subl._{0.01}$ 150°. Diamagnetic.

Johnson, B.F.G., *J. Chem. Soc. A*, 1969, 1668 (*cryst struct, nmr, ir*)
Herberhold, M. *et al*, *Chem. Ber.*, 1983, **116**, 2896 (*ir, pmr*)

$C_6H_{13}O_9S_3Yb$ IC-005248

Ytterbium(*III*) ethylsulfate

$Yb[OS(O)_2Et]_3$

M 500.4
Obt. as nonahydrate.
Nonahydrate: [56422-18-5]. *Nonaaquaytterbium(3+) tris(ethylsulfate)*
Colourless cryst. Sol. H_2O. Contains $[Yb(OH_2)_9]^{3\oplus}$ ions (tricapped trigonal prismatic).

Cooke, A.H. *et al, Philos. Mag.*, 1957, **2**, 928 (*magnetism*)
Staveley, L.A.K. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
Albertsson, J. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 1460 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl.*, 1981, **C8**, 362 (*rev*)

$C_6H_{15}PS_3$ IC-005249

Triethyl phosphorotrithioite, 9CI

Triethyl trithiophosphite. Tri(ethylthio)phosphorus(III)

[688-62-0]

$(EtS)_3P$

M 214.3
Ligand for Hg and Au. Liq. d_4^{25} 1.16. Mp −32°. Bp_{18} 140-143°.

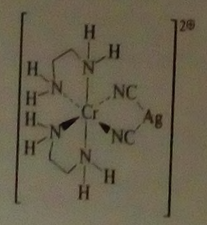
▷ TG5700000.

B,MeI: Tri(ethylthio)methylphosphonium iodide
$C_7H_{18}IPS_3$ M 356.2
Solid. Mp 191°.
B,EtI: Ethyltri(ethylthio)phosphonium iodide
$C_8H_{20}IPS_3$ M 370.3
Solid. Mp 125-127°.

Lippert, A. *et al, J. Am. Chem. Soc.*, 1938, **60**, 2370 (*synth, derivs*)
Chernova, A.V. *et al, Zh. Obshch. Khim.*, 1979, **49**, 2002; *J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 1760 (*uv, struct*)
Kostin, V.P. *et al, Zh. Obshch. Khim.*, 1982, **52**, 498, 2698; *J. Gen. Chem. USSR (Engl. Transl.)*, 1982, **52**, 437, 2379 (*synth, P-31 nmr*)
Zverev, V.V. *et al, Zh. Obshch. Khim.*, 1983, **53**, 1968; *J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 1775 (*pe*)
Nifant'ev, E.E. *et al, Zh. Obshch. Khim.*, 1983, **53**, 2695; *J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 2429 (*synth, P-31 nmr*)
Filippova, E.A. *et al, Zh. Prikl. Spektrosk.*, 1987, **46**, 761; *J. Appl. Spectrosc. USSR (Engl. Transl.)*, 1987, **46**, 467 (*ir, raman*)

$C_6H_{16}AgCrN_6^{2\oplus}$ IC-005250

Bis(cyano-*N*)bis(1,2-ethanediamine-*N,N'*) silverchromium(2+)



M 332.0 (ion)

cis-form

Linkage isomer of *cis*-$[Cr(CN)_2(en)_2]^{\oplus}$ formed through interaction with $Ag^{\oplus}$ (see also Bis[dicyanosilver(*I*)-*N*]bis(ethylenediamine)chromium(*III*), IC-006053). Precipitation of AgI regenerates uv spectrum of *cis*-$[Cr(CN)_2(en)_2]^{\oplus}$.

Diperchlorate: [75047-20-0].

Synth. from $AgNO_3$ and *cis*-$[Cr(CN)_2(en)_2]ClO_4$ followed by $NaClO_4$. Yellow orange solid.

Heatherington, A. *et al, Inorg. Chim. Acta*, 1980, **44**, L279 (*synth, uv, ir*)

$C_6H_{16}AlNaO_4$ IC-005251

Sodium dihydrobis(2-methoxyethanolato-*O,O'*) aluminate(1−)

Sodium bis(2-methoxyethoxy)aluminium hydride. RED-Al. SDMA. Vitride. Synhydride

[22722-98-1]

$NaAlH_2(OCH_2CH_2OMe)_2$

M 202.1
Oligomeric structs. proposed in soln. Widely used as reducing agent in org. chem. Viscous moisture sensitive liq. Used as 70% soln. in toluene. Sol. hydrocarbons, ethers. ΔH_f −1316 kJ mol^{-1}.

Walker, E.R.H., *Chem. Soc. Rev.*, 1976, **5**, 23 (*use*)
Inorg. Synth., 1978, **18**, 149 (*synth*)
Štrouf, O. *et al, J. Organomet. Chem. Libr.*, 1985, **150** (*rev, props, use*)
Heřmánek, S. *et al, Z. Naturforsch., B*, 1985, **40**, 582 (*Al-27 nmr*)
Vit, J., *HEXCEL Corporation Technical Information Bull.*, 1986 (*rev, use*)

$C_6H_{16}AlO_2^{\ominus}$ IC-005252

Dihydrodiisopropoxyaluminate(1−)

Dihydrobis(2-propanolato)aluminate(1−)

$[AlH_2[OCH(CH_3)_2]_2]^{\ominus}$

M 147.1 (ion)
Detected in soln. by nmr as Me_4N salt.

Li salt: [70556-31-9].
Shown to be a mixt. of $LiAlH_4$ and $LiAl[OCH(CH_3)_2]_4$.

Turova, N.Ya. *et al, Zh. Obshch. Khim.*, 1977, **47**, 1338; *Inorg. Chim. Acta*, 1977, **21**, 157 (*synth, powder struct*)
Heřmánek, S. *et al, Z. Naturforsch., B*, 1987, **42**, 539 (*Al-27 nmr*)

$C_6H_{16}AlO_3^{\ominus}$ IC-005253

Triethoxyhydroaluminate(1−)

$[AlH(OEt)_3]^{\ominus}$

M 163.1 (ion)

Li salt: [17250-30-5].
Synth. from $LiAlH_4$ and 3EtOH in Et_2O. Selective reducing agent. White moisture-sensitive solid. May be assoc. in soln.

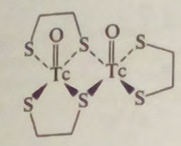
Brown, H.C. *et al, J. Am. Chem. Soc.*, 1964, **86**, 1089 (*synth, use*)
Haubenstock, H., *J. Org. Chem.*, 1973, **38**, 1765 (*use*)
Peretti, D. *et al, Bull. Soc. Chim. Fr.*, 1974, 2925 (*use*)
Turova, N.Ya., *Inorg. Chim. Acta*, 1977, **21**, 157 (*synth, powder struct*)
Turova, N.Ya. *et al, Zh. Obshch. Khim.*, 1977, **47**, 1338 (*props, powder struct*)
Gavrilenko, V.V. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1979, **28**, 1273 (*Al-27 nmr*)
Gless, R.D. *et al, J. Org. Chem.*, 1979, **44**, 1324 (*use*)
Hermanek, S. *et al, Z. Naturforsch., B*, 1987, **42**, 539 (*ir*)

$C_6H_{13}O_5S_6Tc_2$ IC-005161

Tris[1,2-ethanedithiolato(2−)-*S,S'*]dioxoditechnetium(*V*)

Bis[μ-[1,2-ethanedithiolato(2−)-S:S,S']][1,2-ethanedithiolato(2−)-S,S']dioxoditechnetium, 11CI

[96241-63-3]



M 506.3
Synth. from $[Bu_4N][TcOCl_4]$ and limited amount of ethanedithiol in MeOH. Monoclinic orange blocks, gives Bis[1,2-ethanedithiolato(2−)-*S,S'*]oxotechnetate(*V*)(1−), IC-004097 with an excess of ethanedithiol.

[86119-88-2]

De Pamphilis, B.V. *et al, Inorg. Chem.*, 1983, **22**, 2292 (*synth*)
Davison, A., *Technetium in Chemistry and Nuclear Medicine*, Ed. Deutsch, E. *et al*, Cortina International, Verona, 1983, 3 (*synth, cryst struct*)
Davison, A. *et al, Can. J. Chem.*, 1985, **63**, 319 (*synth, struct*)

$C_6H_{12}O_4$ IC-005162

Tetramethoxyethene

Tetramethoxyethylene

$(MeO)_2C{=}C(OMe)_2$

M 148.1
Bp_{15} 48°. n_D^{20} 1.4244.

▷ Prepn. explosive on large scale.

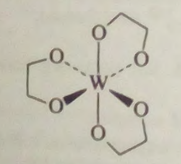
Hoffmann, R.W. *et al, Tetrahedron*, 1965, **21**, 891 (*synth, pmr*)
Scheeren, J.W. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1973, **92**, 11 (*synth*)
Herberhold, M. *et al, Z. Naturforsch., B*, 1976, **31**, 35 (*pmr, cmr*)
Kopecky, K.R. *et al, Can. J. Chem.*, 1988, **66**, 2234.

$C_6H_{12}O_6W$ IC-005163

Tris[1,2-ethanediolato(2−)-*O,O'*]tungsten(*VI*), 9CI

Tris(ethylene-1,2-dioxo)tungsten(VI)

[54153-67-2]



M 364.0
Octahedral. Interatomic distance: W—O 190.8 pm. Cryst. Forms a monohydrate.

[42592-41-6]

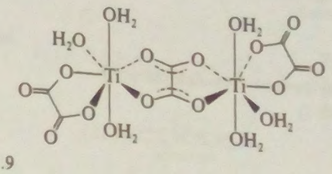
Scherle, J. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 2772 (*cryst struct*)

$C_6H_{12}O_{18}Ti_2$ IC-005164

Hexaaqua-μ-oxalatobis(oxalato)dititanium(*III*)

μ-Oxalatobis[oxalatotriaquotitanium(III)]. *Hexaaqua[μ-[ethanedioato(2−)-O,O''':O',O'']]bis[ethanedioato(2−)-O,O']dititanium*(III), *10CI*

[24436-22-4]

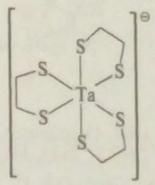


M 467.9
Linked pentagonal bipyramids. Magnetic measurements show significant exchange although the titaniums are well separated. Synth. from $TiCl_3$ and oxalic acid in aq. soln. Brown solid. Sol. H_2O, insol. EtOH. Paramagnetic, $\mu_{eff} = 1.54\mu_B$ (295K). The temp. dependence indicates J = −60 cm^{-1}.

Eve, D.J. *et al, J. Chem. Soc. A*, 1966, 1183 (*synth, ir, uv, magnetism*)
Drew, M.G.B. *et al, J. Chem. Soc., Dalton Trans.*, 1969, 876 (*cryst struct, uv-vis*)
Wrobleski, J.T. *et al, Inorg. Chim. Acta*, 1980, **38**, 227 (*magnetism, uv-vis*)

$C_6H_{12}S_6Ta^{\ominus}$ IC-005165

Tris[1,2-ethanedithiolato(2−)-*S,S'*]tantalate(*V*)(1−), 11CI



M 457.5 (ion)
Prob. like the Nb analogue: a struct. intermediate between octahedral and trigonal prismatic.

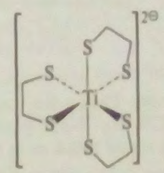
Et_4N salt: [99797-22-5].
Synth. from $TaCl_5$, $LiSCH_2CH_2SLi$ and $[Et_4N]Cl$ in MeCN. Orange solid.

Tatsumi, K. *et al, Angew. Chem., Int. Ed. Engl.*, 1986, **25**, 86 (*synth, ir, uv-vis, pmr*)

$C_6H_{12}S_6Ti^{2\ominus}$ IC-005166

Tris(1,2-ethanedithiolato-*S,S'*)titanate(*IV*)(2−), 11CI

[94750-77-3]



M 324.4 (ion)
Octahedral but distorted towards trigonal prismatic geometry.

Bis-Et_4N salt: [94750-78-4].

Synth. from $Na_2S_2C_2H_4$, $TiCl_4$ and Et_4NCl in MeCN, or from $TiCl_3$, Et_4NBr and $Na_2S_2C_2H_4$ in MeCN. Orange, diamagnetic air-sensitive cryst. Sol. MeCN, Et_2O.

Dorfman, J.R. *et al*, *Inorg. Chem.*, 1985, **24**, 453 (*synth, cryst struct, uv-vis, Et_4N salt*)
Rao, C. *et al*, *Inorg. Chem.*, 1986, **25**, 428 (*synth, struct, uv-vis*)
Mukherjee, R.N. *et al*, *Inorg. Chem.*, 1986, **25**, 2979 (*uv-vis, electrochem*)

IC-005167

$C_6H_{13}AgS$

(3-Methylpentane-3-thiolato)silver(*I*)

[87337-48-2]

$AgSC(CH_3)(CH_2CH_3)_2$

M 225.1
Struct. comprises chains of silver and sulfur atoms. Each chain contains 2 separate and unconnected $(Ag—SR)_\infty$ strands. Colourless cryst. Sol. CCl_4, $CHCl_3$, C_6H_6, toluene, pet. ether, Et_2O, THF,warm EtOH, warm Me_2CO. Mp 145-146°.

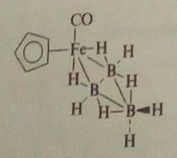
Dance, I.G. *et al*, *Inorg. Chem.*, 1983, **22**, 3785 (*cryst struct, synth, pmr*)

IC-005168

$C_6H_{17}B_3FeO$

Carbonyl(η⁵-2,4-cyclopentadien-1-yl)[octahydrotriborato(1 –)]iron

[53802-00-9]



M 189.4
Dark brown -black solid. Deep purple, air-sensitive soln. in hydrocarbons, CH_2Cl_2, Et_2O, Me_2CO. Mp 53-54°.

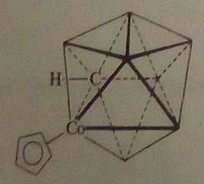
Gaines, D.F. *et al*, *Inorg. Chem.*, 1978, **17**, 794 (*synth, ms, pmr, B-11 nmr, ir*)

IC-005169

$C_6H_{13}B_7Co$

(η⁵-2,4-Cyclopentadien-1-yl)[(3,4,5,6,8-η)-octahydro-4-carbaoctaborato(3 –)]cobalt, 9CI

[38882-81-4]



M 219.7
Proposed struct. shown. Dark green (nearly black) solid. Sol. CH_2Cl_2, MeCN. Mp 79-81°. Paramagnetic. Heat sensitive, must be stored below or at 0°.

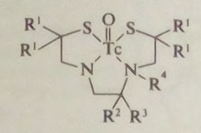
Dustin, D.F. *et al*, *Inorg. Chem.*, 1973, **12**, 1380 (*synth, ir, ms*)

$C_6H_{13}N_2OS_2Tc$

IC-005170

Oxo[1,1′-[1,2-ethanediyl]diimino]bis[ethanedithiolato](3 –)]technetium

Diaminodithiolatooxotechnetium(V).
Bisaminoethanethiol—Tc. DADT—Tc. BAT—Tc



$R^1 = R^2 = R^3 = R^4 = H$

M 292.2
Simplest form of important series of potential pharmaceuticals with $TcO(S_2N_2)$ core. R_1 and R_2 generally H or Me, but can also be Et, cyclohexyl, etc.; R_3 = H, Me, CH_2OH, CH_2NH_2, C_6H_4OH, C_6H_4OMe, various piperidine derivatives; R_4 generally H.

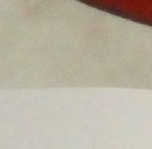
Kung, H.F. *et al*, *J. Nucl. Med.*, 1984, **25**, 16, 128, 326 (*analogues, synth, partition coeff, biodistrib, hplc, electrophoresis*)
Baidoo, K.E. *et al*, *J. Nucl. Med.*, 1987, **28**, 729 (*analogues, partition coeff*)
Scheffel, U. *et al*, *J. Nucl. Med.*, 1988, **29**, 73 (*analogues, synth, lipophilicity*)

$C_6H_{14}As_2Cl_2Ni$

IC-005171

Dichloro[1,2-ethenediylbis[dimethylarsine]-*As,As′*]nickel(*II*)

Dichloro[vinylenebis(dimethylarsine)]nickel(II), *8CI*. *[1,2-Bis(dimethylarsino)ethene]dichloronickel*(II)



cis-form

M 365.6
cis-ligand gives planar monomer; *trans*- gives octahedral polymer with coordinated EtOH. Complexes with other anions and $[ML_2]^{2\oplus}$ also formed.

cis*$_{ligand}$-*form
Pale brown solid. Sol. polar org. solvs.

trans*$_{ligand}$-*form
Forms as 2EtOH complex.

Bis-EtOH complex: catena-*Dichlorobis(ethanol)[1,2-ethenediylbis[dimethylarsine]]nickel*
$C_{10}H_{26}As_2Cl_2NiO_2$ M 457.7
Green cryst. Sol. polar solvs. Paramagnetic.

Bennett, M.A. *et al*, *J. Chem. Soc. A*, 1971, 536 (*synth, ir, magnetism*)

$C_6H_{14}BBr_3S$

IC-005172

Tribromo(dipropyl sulfide)boron

Tribromo[1,1′-thiobis[propane]]boron, 10CI. Tribromoborane compd. with 1,1′-thiobis[propane] (*1:1*). *Boron tribromide dipropyl sulfide. Tribromoborane dipropyl sulfide*

[61552-15-6]

$(H_3CCH_2CH_2)_2S—BBr_3$

M 368.7

Romm, I.P. *et al*, *Zh. Obshch. Khim.*, 1976, **46**, 2445.

Gol'dshtein, I.P. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **237**, 1392.
Gol'dshtein, I.P. *et al*, *Zh. Obshch. Khim.*, 1978, **48**, 2568.
Gol'dshtein, I.P. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1980, **252**, 909.

IC-005173

$C_6H_{14}BBr_3Se$

Tribromo(dipropyl selenide)boron

Tribromo[1,1′-selenobis[propane]]boron, 10CI.
Tribromoborane compd. with 1,1′-selenobis[propane] (*1:1*).
Boron tribromide dipropyl selenide. Tribromoborane dipropyl selenide

[65907-94-0]

$(H_3CCH_2CH_2)_2Se—BBr_3$

M 415.6

Gol'dshtein, I.P. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **237**, 1392; 1980, **252**, 909.
Gol'dshtein, I.P. *et al*, *Zh. Obshch. Khim.*, 1978, **48**, 2568.

IC-005174

$C_6H_{14}BiCl_2O_2PS_2$

1,1-Dichloro-5-methyl-3-(1-methylethoxy)-4-oxa-2-thia-3-phospha-1-bismahexane 3-sulfide, 11CI

Dichloro[(diisopropoxyphosphinothioyl)thio]bismuthine. S-Dichlorobismuthino-O,O-diisopropylphosphorodithioate

[89928-32-5]

$[(H_3C)_2CHO]_2P(S)SBiCl_2$

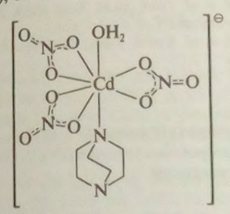
M 493.1
Yellow cryst. Mp 138°.

Chauhan, H.P.S. *et al*, *Phosphorus Sulfur*, 1983, **17**, 161.

IC-005175

$C_6H_{14}CdN_5O_{10}^{\ominus}$

Aqua(1,4-diazabicyclo[2.2.2]octane-*N*)tris(nitrato-*O,O′*)cadmate(1 –), 11CI



M 428.6 (ion)
Hexagonal bipyramidal anion.

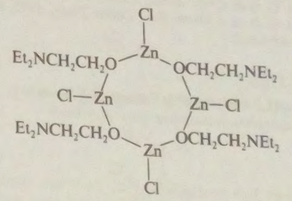
H compd.: [89230-26-2]. *Aqua(4-aza-1-azoniabicyclo[2.2.2]octane)trinitratocadmium*
Cryst. (aq. MeOH). Sol. H_2O.

Viossat, B. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 24 (*synth, cryst struct*)

$C_6H_{14}ClNOZn$

IC-005176

Chloro[2-(diethylamino)ethanolato]zinc



tetramer

M 217.0
Tetrameric. Analogous bromo compd. also prepd.
Tetramer: [55428-26-7]. *Tetrachlorotetrakis[μ-[2-(diethylamino)ethanolato-N,O:O]]tetrazinc, 9CI*
$C_{24}H_{56}Cl_4N_4O_4Zn_4$ M 868.1
Cryst. (EtOH).

Haase, W. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1184 (*synth, cryst struct*)

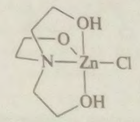
$C_6H_{14}ClNO_3Zn$

IC-005177

Chloro[[2,2′,2″-nitrilotris[ethanolato]](1 –)-*N,O,O′,O″*]zinc, 9CI

Chloro[tris(ethanol)aminato]zinc

[33520-38-6]



M 249.0
Mod. air-stable, hygroscopic white cryst. (EtOH). Sl. sol. alcohols. Mp 232-236°. Hydrol. in aq. soln.

Garelli, F. *et al*, *Gazz. Chim. Ital.*, 1933, **63**, 570 (*synth*)
Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1934, **219**, 225 (*synth*)
Sen, B. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 2707 (*synth, ir*)
Follner, H. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 157 (*cryst struct*)

IC-005178

$C_6H_{14}ClN_2O_5Re$

Chlorobis(*N,N*-dimethylformamide-*O*)trioxorhenium(*VII*)

Rhenium chloride trioxide bis(dimethylformamide)

[19584-29-3]

$ReO_3Cl(HCONMe_2)_2$

M 415.8
Synth. e.g. from ReO_3Cl and DMF. Yellow, hygroscopic cryst. Sol. CH_2Cl_2, DMF, $CHCl_3$, EtOH; insol. Et_2O, C_6H_6, CCl_4. Dec. at 140°.

Ringel, C. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **353**, 158 (*synth, ir, props*)
Gerlach, U. *et al*, *Z. Chem.*, 1977, **17**, 305 (*synth, ir*)

IC-005179

$C_6H_{14}Cl_2HgN_2O_2S_2$

Dichlorobis(*O*-ethyl thiocarbamate)mercury

Dichlorobis(O-ethyl carbamothioate-S)mercury, 9CI

[53140-35-5]

$[EtOC(NH_2)=S]_2HgCl_2$

M 481.8

Hydrogen bonded 3-D network in solid state. Cryst. (Me_2CO/pet. ether). Mp 105-107°.

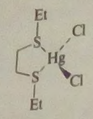
Bandoli, G. *et al*, *Cryst. Struct. Chem.*, 1974, **3**, 289 (*cryst struct*)
Bandoli, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 449 (*synth, ir, cryst struct*)

IC-005180

$C_6H_{14}Cl_2HgS_2$

Dichloro[1,2-bis(ethylthio)ethane-*S,S'*]mercury

[1,2-Bis(ethylthio)ethane]mercury dichloride



M 421.8
Solid. Mp 99-100°.

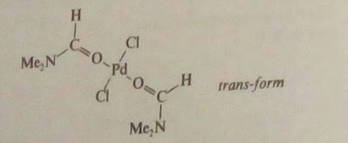
Shostakovskii, M.F., *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1954, 526 (*synth*)
Coates, G.E. *et al*, *J. Chem. Soc.*, 1964, 166 (*synth, ir*)

IC-005181

$C_6H_{14}Cl_2N_2O_2Pd$

Dichlorobis(dimethylformamide)palladium(*II*)

[34730-99-9]



trans-form

M 323.5
Ir indicates O-coordination and *trans*-struct. for only known isomer. Synth. from $PdCl_2$ and DMF. Brown powder, dissoc. in CH_2Cl_2 soln. Insol. CCl_4, Et_2O, isopentane; sol. CH_2Cl_2, 1,2-dichloroethane. Ir ν_{Pd-O} 429 cm^{-1} (nujol).

[20589-35-9, 53649-60-8]

Wayland, B.B. *et al*, *Inorg. Chem.*, 1969, **8**, 971 (*synth, ir*)
Gioria, J.M. *et al*, *Helv. Chim. Acta*, 1971, **54**, 2251 (*synth, props, ir*)

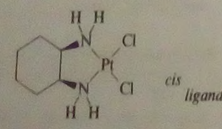
IC-005182

$C_6H_{14}Cl_2N_2Pt$

Dichloro(1,2-cyclohexanediamine-*N,N'*)platinum, 9CI

Dichloro(1,2-diaminocyclohexane)platinum(II)

[52691-24-4]



cis ligand -form

M 380.1
Much investigated for antitumour prop. Useful intermed. for other complexes by reaction with Ag salts. Yellow cryst. Sol. polar solvs.

▷ TP2275974.

cis*-$_{R,R}$-*form [61848-70-2]
meso-*form*
Pale yellow cryst. + ½ H_2O. Sol. DMF. Ir ν_{NH} 3250s, 3195s, 3125s; ν_{PtCl} 325 cm^{-1} (nujol).
▷ TP2275992.

1S-trans*-$_{R,R}$-*form [61848-62-2]
(+)-*form*
Synth. from $PtCl_2(DMSO)_2$ and *S,S*-1,2-diaminocyclohexane. Sol. DMF.

1R-trans*-$_{R,R}$-*form [61848-66-6]
(−)-*form*
Bright yellow solid. Sol. DMF.
▷ TP2275980.

(±)-***trans*-$_{R,R}$-*form*** [38780-40-4]
▷ TP2492220.

[77057-09-1]

Lock, C.J.L. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 45 (*synth, cryst struct, cis-form*)
Gullotti, M. *et al*, *Inorg. Chim. Acta*, 1984, **91**, 223 (*antitumour props*)
Fanizzi, F.P. *et al*, *Inorg. Chim. Acta*, 1987, **137**, 45 (*mutagenicity*)
Vollano, J.F. *et al*, *J. Med. Chem.*, 1987, **30**, 716 (*synth, props, antitumour props*)

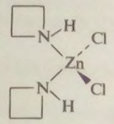
IC-005183

$C_6H_{14}Cl_2N_2Zn$

Bis(azetidine)dichlorozinc

Bis(azetidine)zinc dichloride. *Zinc*(II) *chloride bis(azetidine)*

[53293-48-4]



M 250.4
Needles (EtOH). Ligand polymerises on heating compd.

Razumova, E.P. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1974, 515 (*synth, ir, raman*)
Ledina, L.E. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1980, **255**, 874 (*synth, ir, pmr*)
Perchenko, V.N. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1981, **261**, 114 (*thermal anal*)
Perchenko, V.N. *et al*, *Koord. Khim.*, 1985, **11**, 161 (*synth, ir, thermal anal*)

IC-005184

$C_6H_{14}Cl_2O_2Ti$

Dichlorodiisopropoxytitanium(*IV*), 8CI

Dichlorobis(2-propanolato)titanium(IV), *11CI. Titanium*(IV) *dichloride diisopropoxide*

[762-99-2]

$$[(H_3C)_2CHO]_2TiCl_2$$

M 236.9
Tetrahedral. Synth. from $TiCl_4$ and $(i\text{-}PrO)_2SiMe_2$ in hexane. Widely used in catalysts for olefin polym. and many other reactions.

Dijkgraaf, C. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 1213 (*ir*)
Czaja, K. *et al*, *Polimery (Warsaw)*, 1984, **29**, 411 (*use*)
Ger. Pat., 3 447 297, (1986); *CA*, **105**, 175282g (*synth, use*)

IC-005185

$C_6H_{14}Cl_2O_2Ti$

Dichlorodipropoxytitanium(*IV*), 11CI

Dichlorobis(propanolato)titanium(IV). *Titanium*(IV) *dichloride dipropoxide*

[1790-23-4]

$$(H_3CCH_2CH_2O)_2TiCl_2$$

M 236.9

Tetrahedral. Synth. from $TiCl_4$ and $(H_3CCH_2CH_2O)_2SiMe_2$ in hexane. Used widely in olefin polym. catalysts but not for other reactions (cf Dichlorodiisopropoxytitanium(*IV*), IC-005184); component of photosensitive colour-forming solns.

U.S. Pat., 4 173 521, (1969); *CA*, **92**, 155914z (*photosensitive solns*)
Fr. Pat., 2 566 782, (1986); *CA*, **105**, 61079r (*use, polym*)
Ger. Pat., 3 447 297, (1986); *CA*, **105**, 175282g (*synth, use, polym*)

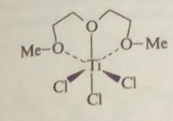
IC-005186

$C_6H_{14}Cl_2O_3Ti$

Trichloro[1,1'-oxybis[2-methoxyethane]-*O,O',O'*]titanium(*III*), 10CI

Trichloro(2,5,8-trioxanonane)titanium(III). *Trichloro(diglyme)titanium*(III). *Titanium*(III) *chloride diglyme*

[69178-49-0]



M 288.4
fac-Octahedral. Synth. by reaction of $TiCl_3$, benzoic acid and benzoic anhydride in diglyme. The product is adventitious and is *not* formed by reaction of $TiCl_3$ and diglyme. V. air and moisture sensitive solid.

Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1176 (*cryst struct, synth*)

IC-005187

$C_6H_{14}Cl_4N_2O_2Ti$

Tetrachlorobis(*N,N*-dimethylformamide-*O*)titanium(*IV*), 11CI

Titanium(IV) *chloride bis(dimethylformamide)*

[12106-37-5]

$$(Me_2NCHO)_2TiCl_4$$

M 335.8
Octahedral. Detailed geometry not known. Synth. by adding DMF to a soln. of $TiCl_4$ in CH_2Cl_2 until precipitation is complete. Used in pre-treatment of poly(acrylonitrile) fibres for carbon fibre manuf. Insol. CH_2Cl_2.

Ger. Pat., 2 016 445, (1971); *CA*, **76**, 114699j (*use*)
Doron, V. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 889 (*synth, cd*)
Kuz'min, A.I. *et al*, *Koord. Khim.*, 1982, **8**, 159; *CA*, **96**, 154238c (*nqr*)

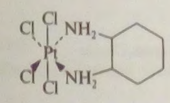
IC-005188

$C_6H_{14}Cl_4N_2Pt$

Tetraplatin

*Tetrachloro(1,2-cyclohexanediamine-*N,N'*)platinum*

[62816-98-2]



M 451.0
Antineoplastic agent.

▷ TP2282000.

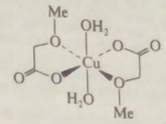
[96392-95-9, 96392-96-0, 96392-97-1]

Schwartz, P. *et al*, *Cancer Treat. Rep.*, 1977, **61**, 1519 (*synth*)
Gale, G.R. *et al*, *Bioorg. Chem.*, 1978, **8**, 495 (*pharmacol*)
Anderson, W.K. *et al*, *Cancer Treat. Rep.*, 1986, **70**, 997 (*synth, stom*)

$C_6H_{14}CuO_8$

Diaquabis(methoxyacetato-O^1,O^2)copper(*II*), 9CI IC-005189

[22239-89-0]



M 277.7
Tetragonally distorted CuO_6 octahedron with two short and four long bonds. Pale blue cryst.

Forrest, J.G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 658 (*magnetism, cryst struct*)
Prout, C.K. *et al*, *J. Chem. Soc. A*, 1968, 2791 (*cryst struct, synth*)
Bew, M.J. *et al*, *J. Chem. Soc. A*, 1970, 2640 (*uv, esr*)
Dawson, K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1509 (*esr*)
Fischinger, A.J., *Appl. Spectrosc.*, 1973, **27**, 58 (*synth*)
Hitchman, M.A., *J. Chem. Soc., Faraday Trans. 2*, 1976, **72**, 54 (*uv, theory*)

IC-005190

$C_6H_{14}FN_2O_5Re$

Bis(*N,N*-dimethylformamide-*O*)fluorotrioxorhenium(*VII*)

Rhenium fluoride trioxide bis(dimethylformamide)

[64539-33-9]

$$ReO_3F(HCONMe_2)_2$$

M 399.3
Synth. from Re_2O_7 and HF in DMF. Yellowish, hygroscopic cryst. Mp 124-139°.

Gerlach, U. *et al*, *Z. Chem.*, 1977, **17**, 306 (*synth, ir, props*)

IC-005191

$C_6H_{14}LiN$

Lithium diisopropylamide

LDA. N-*Lithiodiisopropylamine*. *Diisopropylamine lithium salt*. *Bis(1-methylethyl)aminolithium*. N-(*1-Methylethyl*)-2-*propanamine lithium salt, 9CI*

[4111-54-0]

$$LiN[CH(CH_3)_2]_2$$

M 107.1
V. useful, relatively nonnucleophilic strong base used for generation of carbanions. Can function as single electron donor or as hydride donor. Commercially available as solid or suspended in hexanes (10 wt%). Solid. Sol. ethers, insol. or spar. sol. hydrocarbons. Cleaves ethers rapidly at 0° or above, but solns. in eg. 1:1 THF-cyclohexane are much more stable. Complex with enolate descr.

▷ Pyrophoric; corrosive.

Dimer, complex with enolate of 3,3-dimethyl-5-(dimethyl-tert-butylsilyloxy)pentan-2-one: [110015-47-9]. *Bis*[μ_3-[5-[[(*1,1-dimethylethyl*)*dimethylsilyl*]*oxy*]-*3,3-dimethyl-1-penten-2-olato-*O^1:O^1:O^1,O^3]]*bis*[μ-[N-(*1-methylethyl*)-2-*propanaminato*]]*tetralithium*
$C_{38}H_{82}Li_4N_2O_4Si_2$ M 715.0
Large transparent cryst. (heptane).

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 249; **3**, 184; **4**, 298; **5**, 400; **6**, 334; **7**, 204; **8**, 292; **9**, 280; **10**, 241; **11**, 296 (*uses*)
Carey, F.A. *et al*, *J. Org. Chem.*, 1976, **41**, 3979 (*rev*)
House, H.O. *et al*, *J. Org. Chem.*, 1978, **43**, 700 (*synth, stability*)
Lochmann, L. *et al*, *J. Organomet. Chem.*, 1979, **179**, 123 (*ir*)
Reetz, M.T. *et al*, *Justus Liebigs Ann. Chem.*, 1980, 1471 (*synth*)

Williard, P.G. *et al, J. Am. Chem. Soc.*, 1987, **109**, 5539 (*deriv, cryst struct*)
Kopka, I.E. *et al, J. Org. Chem.*, 1987, **52**, 448 (*synth, props*)
Einhorn, J. *et al, J. Org. Chem.*, 1987, **52**, 4124 (*synth*)
Brandsma, L. *et al, Prep. Polar Organometallic Chemistry*, Springer-Verlag, Berlin, 1987, **1** (*synth*)
Shiner, C.S. *et al, J. Am. Chem. Soc.*, 1988, **110**, 957 (*props*)
Renaud, P. *et al, J. Am. Chem. Soc.*, 1988, **110**, 5702 (*polarog, props*)
Podraza, K.F. *et al, J. Org. Chem.*, 1988, **53**, 2642 (*synth, cmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2154C, 2154D.
Majewski, M. *et al, Tetrahedron Lett.*, 1988, **29**, 4057 (*props*)

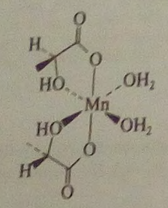
IC-005192

$C_6H_{14}MnO_6$

Diaquabis(2-hydroxypropanoato-O^1,O^2)manganese, 11Cl

Diaquabis(L-lactato)manganese(II)

[18475-79-1]



M 269.1
cis-Octahedral struct. Synth. from $MnCO_3$ and L-lactic acid. Nearly colourless cryst.

Lis, T., *Acta Crystallogr., Sect. B*, 1982, **38**, 937 (*synth, cryst struct*)

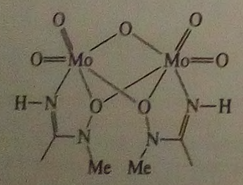
IC-005193

$C_6H_{14}Mo_2N_4O_7$

μ-Oxobis[(*N*-hydroxy-*N*-methylacetamidinato-*N*′,*O*)*cis*-dioxomolybdenum(*VI*)]

Bis[μ-(N-hydroxy-N-methylethanimidamidato-N′,O:O)]-μ-oxotetraoxodimolybdenum(VI), *10Cl*

[79110-78-4]



M 446.0
Air-stable yellow cryst.

Wieghardt, K. *et al, Chem. Ber.*, 1981, **114**, 2700 (*cryst struct, synth, pmr*)

IC-005194

$C_6H_{14}NNa$

Sodium diisopropylamide

N-Sodiodiisopropylamine. Bis(1-methylethyl)aminosodium. N-(1-Methylethyl)-2-propanamine sodium salt, 9CI

[72316-19-9]

$NaN[CH(CH_3)_2]_2$

M 123.1
Solid. Almost insol. C_6H_6.

Lochmann, L. *et al, J. Organomet. Chem.*, 1979, **179**, 123 (*synth, props, ir*)

IC-005195

$C_6H_{14}NO_3Re$

(Diisopropylamino)trioxorhenium(*VII*)

[N-(1-Methylethyl)-2-propanaminato]trioxorhenium, 11Cl

[95544-44-8]

$[(H_3C)_2CH]_2NReO_3$

M 334.3
Synth. from ReO_3Cl and diisopropylamine in hydrocarbon solvs. Pale yellow crystalline solid, volatile, moisture sensitive and thermally unstable at r.t. V. sol. many org. solvs. Mp ~30°. $\nu_{Re=O}$ 989, 950 cm^{-1}.

Edwards, P. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2695 (*synth, ir, nmr, struct, props*)

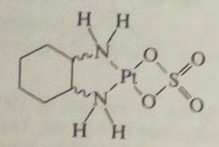
IC-005196

$C_6H_{14}N_2O_4PtS$

(Cyclohexane-1,2-diamine)sulfatoplatinum(*II*), 10Cl

(1,2-Diaminocyclohexane)sulfatoplatinum(II)

[61593-75-7]



M 405.3
Configuration confers chirality. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + $C_6H_{10}(NH_2)_2$, Ag_2SO_4. One of many $C_6H_{10}(NH_2)_2$-Pt(*II*) complexes studied for antitumour properties. Appearance not descr.

[62011-40-9, 66900-70-7, 66900-71-8]

Meischen, S.J. *et al, J. Natl. Cancer Inst. (U.S.)*, 1976, **57**, 841.

IC-005197

$C_6H_{14}N_4O_4S_2Zn$

Bis(acetato-*O*)bis(thiourea-*S*)zinc

Bis(thiourea-S)zinc diacetate

[15377-12-5]

$Zn(OAc)_2[S=C(NH_2)_2]_2$

M 335.7
Essentially tetrahedral Zn (2O + 2S) with two additional weaker intramolecular oxygen contacts. Cryst. (H_2O). Mp 185°. Dec. at *ca.* 200-250° to ZnS.

[59927-00-3]

Nardelli, M. *et al, Ric. Sci.*, 1959, **29**, 1731 (*synth*)
Cavalea, L. *et al, Acta Crystallogr.*, 1967, **22**, 90 (*cryst struct*)
Flint, C.D. *et al, J. Chem. Soc. A*, 1967, 1718 (*ir*)
Druzhinin, I.G. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 246 (*synth*)
Khodzhaev, O.F. *et al, J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 969 (*synth, ir, thermal anal*)

IC-005198

$C_6H_{14}N_4O_6Zn$

Bis(acetato-*O*)bis(urea-*O*)zinc

Di(urea)zinc diacetate. Zinc(II) *acetate bis(urea)*

[52585-07-6]

$Zn(OAc)_2[O=C(NH_2)_2]_2$

M 303.5
Octahedral zinc. Solid. Dec. at 200°.

[59539-59-2]

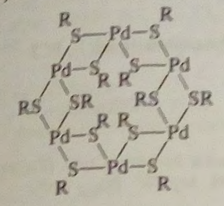
Ergashbaev, Zh. *et al, Izv. Akad. Nauk Kirg. SSR*, 1973, 51; *CA*, 1974, **80**, 59404 (*synth*)
Khodzhaev, O.F. *et al, Koord. Khim.*, 1976, **2**, 304 (*ir, thermal anal*)

IC-005199

$C_6H_{14}PdS_2$

Bis(propanethiolato)palladium(*II*)

Palladium propylmercaptide



R = $CH_2CH_2CH_3$
hexamer

M 256.7
Hexameric; puckered ring struct. of bridging SR groups with approx. square planar Pd.

Hexamer: [35359-97-8]. *Dodecakis[μ-(1-propanethiolato)]hexapalladium*(II), *9CI*
$C_{36}H_{84}Pd_6S_{12}$ M 1540.3
Synth. from Tetrachloropalladate(*II*)(2−), IC-017115 and propanethiol. Pleochroic orange-yellow and yellow, or orange-red needles. Sol. $CHCl_3$, C_6H_6; spar. sol. EtOH, Me_2CO, pet. ether. Mp 209-210°.

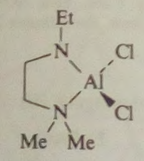
Mann, F.G. *et al, J. Chem. Soc.*, 1935, 1549 (*synth*)
Kunchur, N.R. *et al, Acta Crystallogr., Sect. B*, 1968, **24**, 1623; 1971, **27**, 2292 (*cryst struct*)

IC-005200

$C_6H_{15}AlCl_2N_2$

Dichloro(*N*′-ethyl-*N*,*N*-dimethyl-1,2-ethanediaminato-*N*,*N*′)aluminium, 9CI

[59738-07-7]



M 213.0
Synth. from $AlCl_3$ + $Li[EtNCH_2CH_2NMe_2]$ in toluene. Colourless moisture-sensitive cryst. (toluene). Mp 92-95°. $Subl._{0.01}$ 40°.

Beachley, O.T. *et al, Inorg. Chem.*, 1976, **15**, 2110 (*synth, props, ir, pmr*)
Atwood, J.L. *et al, Inorg. Chem.*, 1980, **19**, 268 (*cryst struct*)

IC-005201

$C_6H_{15}AlO_3$

Aluminum ethoxide

Ethanol aluminum salt, 9CI. Ethyl alcohol aluminum salt, 8CI

[555-75-9]

$Al(OEt)_3$

M 162.1
Mixt. of oligomers in soln. Phys. props. drastically affected by traces of moisture. Reagent for the redn. of carbonyl compds. to alcohols. Catalyst for prepn. of esters from aldehydes and alcoholysis of diketones. Polym. catalyst. Liq. which solidifies to a white glassy solid. Mp ca. 140°. Bp_{4-6} 200°, Bp_1 175-180°.
▷ Highly irritant.

Mehrotra, R.C., *J. Indian Chem. Soc.*, 1953, **30**, 585 (*synth*)
Wilhoit, R.C. *et al, J. Inorg. Nucl. Chem.*, 1962, **24**, 851 (*synth, ir*)
Oliver, J.G. *et al, J. Chem. Soc. A*, 1970, 2347 (*ms*)

IC-005202

$C_6H_{15}AsAuCl$

Chloro(triethylarsine)gold(*I*), 10Cl

[99327-37-4]

$Et_3AsAuCl$

M 394.5
Tested for antitumour props.

Mann, F.G. *et al, J. Chem. Soc.*, 1937, 1828 (*synth*)
Mirabell, C.K. *et al, J. Med. Chem.*, 1986, **29**, 218 (*biol activity*)

IC-005203

$C_6H_{15}AsCl_3Pt^{\ominus}$

Trichloro(triethylarsine)platinate(*II*)(1−), 8Cl

$[PtCl_3(AsEt_3)]^{\ominus}$

M 463.5 (ion)
Square planar struct. Synth. from Tetrachlorobis(triethylarsine)diplatinum(*II*), IC-007999 + $Cl^{\ominus}$. Br, I analogues known.

Tetrapropylammonium salt: [19524-22-2].
Yellow solid. Mp 201°.

Duddell, D.A. *et al, J. Chem. Soc. A*, 1970, 545 (*synth, ir, raman*)
Gosling, R. *et al, Inorg. Chem.*, 1983, **22**, 1235 (*synth, reactions*)

IC-005204

$C_6H_{15}AsCl_5Pd^{\ominus}$

Pentachloro(triethylarsine)palladate(*IV*)(1−)

$[PdCl_5(AsEt_3)]^{\ominus}$

M 445.7 (ion)

Et_4N salt: [83971-09-9].
Moisture-sensitive orange solid.

Gulliver, D.J. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 1896 (*synth, ir, uv-vis*)

IC-005205

$C_6H_{15}AsO_3$

Triethyl arsenite, 9Cl, 8Cl

Arsenous acid triethyl ester, 9Cl, 8Cl. Triethoxyarsine. Triethoxoarsenic

[3141-12-6]

$As(OEt)_3$

M 210.1
Ligand for V. Liq. Bp_4 61°.

Durand, M. *et al, Bull. Soc. Chim. Fr.*, 1969, 48 (*ir, pmr*)
Brill, T.B. *et al, Inorg. Chem.*, 1973, **12**, 1884 (*synth, ir*)
Froeyen, P. *et al, Org. Mass Spectrom.*, 1973, **7**, 73 (*ms*)
Kober, F. *et al, Z. Anorg. Allg. Chem.*, 1973, **403**, 56 (*synth, pmr*)
Zakirov, D.U. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **235**, 1343; *Dokl. Phys. Chem. (Engl. Transl.)*, 1977, **235**, 831.
Baer, C.D. *et al, Inorg. Chem.*, 1983, **22**, 1402 (*reactions*)
Omiadze, A.P. *et al, Zh. Fiz. Khim.*, 1986, **60**, 1575; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1986, **60**, 947 (*props*)

$C_6H_{15}AsO_4$ IC-005206

Triethyl arsenate, 9CI

Arsenic acid triethyl ester, 9CI. Ethyl arsenate

[15606-95-8]

$(EtO)_3As{=}O$

M 226.1
Liq. d_4^{20} 1.31. Bp_9 109°. n_D^{20} 1.4341.

Gallais, F. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1966, **263**, 453 (*synth*)
Laurent, J.P. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 48 (*pmr, ir*)
Froeyen, P. *et al*, *Org. Mass Spectrom.*, 1974, **9**, 132 (*ms*)
Shagidullin, R.R., *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1975, 1677; (*Engl. transl.* p. 1578, 1672), 1977, 1812 (*ir, raman, conform*)
Shagidullin, R.R. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1976, **231**, 1377 (*ir, raman*)
Zakirov, D.U. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, (*Engl. transl.* p. 831), 1977, **235**, 1343 (*nqr*)

$C_6H_{15}AuBrCl_2P$ IC-005207

Bromodichloro(triethylphosphine)gold(*III*), 9CI

[56271-23-9]

$Et_3PAuBrCl_2$

M 465.9
Golden needles (EtOH). More stable than $AuCl_3(PEt_3)$ on standing. Mp 119-120°.

[56213-23-1]

Mann, F.G. *et al*, *J. Chem. Soc.*, 1940, 1235 (*synth*)
Heaton, B.T. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 363 (*P-31 nmr*)

$C_6H_{15}AuBrP$ IC-005208

Bromo(triethylphosphine)gold(*I*), 9CI

[14243-60-8]

$BrAuPEt_3$

M 395.0
Cryst. (EtOH). Sol. $CHCl_3$, C_6H_6, EtOH. Mp 87°.

Mann, F.G. *et al*, *J. Chem. Soc.*, 1940, 1235 (*synth*)
Heaton, B.T. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 363.
McAuliffe, C.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1730 (*rev*)

$C_6H_{15}AuBr_2ClP$ IC-005209

Dibromochloro(triethylphosphine)gold(*III*), 9CI

[56271-24-0]

Et_3PAuBr_2Cl

M 510.3
Dark orange needles (EtOH). Indefinitely stable in solid state. Mp 128-129°.

[56213-24-2]

Mann, F.G. *et al*, *J. Chem. Soc.*, 1940, 1255 (*synth*)
Heaton, B.T. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 363 (*P-31 nmr*)

$C_6H_{15}AuBr_3P$ IC-005210

Tribromo(triethylphosphine)gold(*III*), 11CI, 9CI

[56213-25-3]

Et_3PAuBr_3

M 554.8
Binds specifically at N-7 of guanine in DNA. Red-orange prisms. Sol. toluene, EtOH, $CHCl_3$. Mp 129-131°.

Mann, F.G. *et al*, *J. Chem. Soc.*, 1940, 1235 (*synth*)
Heaton, B.T. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 363 (*nmr*)
McNeillie, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 767 (*pe*)
Eggleston, D.S. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 1357 (*cryst struct*)
Ward, B. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 3810 (*use*)

$C_6H_{15}AuClP$ IC-005211

Chloro(triethylphosphine)gold(*I*), 9CI

[15529-90-5]

$ClAuPEt_3$

M 350.5
Shows antiarthritic activity. Cryst. (EtOH). Sol. C_6H_6, $CHCl_3$, EtOH. Mp 78°. $Bp_{0.03}$ 210°.

▷ MD5431000.

Mann, F.G. *et al*, *J. Chem. Soc.*, 1937, 1828 (*synth*)
Walz, D.T. *et al*, *J. Pharmacol. Exp. Ther.*, 1972, **181**, 292 (*use*)
Schmidbaur, H. *et al*, *Z. Naturforsch., B*, 1976, **31**, 1607 (*nqr*)
Jones, P.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1434 (*mossbauer*)
Puddephatt, R.J. *et al*, *The Chemistry of Gold*, Elsevier, 1978, 248 (*rev*)
McAuliffe, C.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1730 (*synth*)
McNeillie, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 767 (*pe*)

$C_6H_{15}AuCl_3P$ IC-005212

Trichloro(triethylphosphine)gold(*III*), 9CI

[56213-22-0]

Cl_3AuPEt_3

M 421.4
Pale-yellow needles (EtOH). Sol. Me_2CO, $CHCl_3$, spar. sol. EtOH, CCl_4. Mp 121°.

Mann, F.G. *et al*, *J. Chem. Soc.*, 1940, 1235 (*synth*)
Heaton, B.T. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 363 (*nmr*)
Brown, D.H. *et al*, *Inorg. Chim. Acta*, 1979, **32**, 117 (*uv*)
McNeillie, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 767 (*pe*)

$C_6H_{15}AuI_3P$ IC-005213

Triiodo(triethylphosphine)gold(*III*)

Et_3PAuI_3

M 695.8
Mp 77°. Black needles (EtOH). Dec. to black liq. mass on standing for weeks.

Mann, F.G. *et al*, *J. Chem. Soc.*, 1940, 1235 (*synth*)

$C_6H_{15}BF_3N$ IC-005214

Trifluoro(triethylamine)boron

Trifluoroborane triethylamine (1:1). Boron fluoride-triethylamine compd. (1:1), 8CI

[368-37-6]

$F_3B{\cdot}NEt_3$

M 168.9
Colourless cryst.

Gates, P.N. *et al*, *Spectrochim. Acta*, 1965, **21**, 1445 (*synth, pmr, B-11 nmr*)
Davies, P.G. *et al*, *Inorg. Nucl. Chem. Lett.*, 1967, **3**, 249 (*ir*)
Myers, W.H. *et al*, *Inorg. Chem.*, 1975, **14**, 2874 (*synth, pmr*)
Fox, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1275 (*F-19 nmr*)

$C_6H_{15}BF_4O$ IC-005215

Triethyloxonium tetrafluoroborate, 10CI, 9CI

Triethyloxonium fluoroborate

[368-39-8]

$Et_3O^{\oplus}\ BF_4^{\ominus}$

M 189.9
Powerful alkylating agent. Commercially available. Hygroscopic cryst. (Et_2O). Sol. CH_2Cl_2, sl. sol. Et_2O. Mp 91-92° dec.

▷ RR4584700.

Org. Synth., 1966, **46**, 113 (*synth*)
Jones, F.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 927 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 500.

$C_6H_{15}BS_2$ IC-005216

Bis(propylthio)borane, 8CI

Bis(propylmercapto)borane

[15818-68-5]

$(H_3CCH_2CH_2S)_2BH$

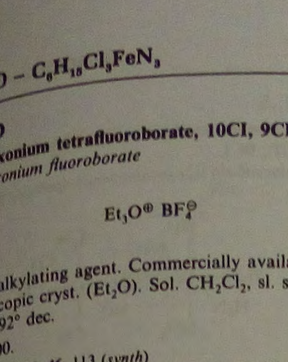
M 162.1
Colourless liq. readily hydrol. in moist air. Sol. Et_2O. d^{20} 0.981. Bp_2 82.5-85°.

Mikhailov, B.M. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1960, 131, 843 (*synth*)
Shchegoleva, T.A. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1963, 443 (*synth, ir*)

$C_6H_{15}B_9Fe^{\ominus}$ IC-005217

(η^5-2,4-Cyclopentadien-1-yl)[η^6-decahydrocarbadecaborato(2−)]ferrate(1−), 10CI

closo-[1-η^5-Cyclopentadienylferrate-2-CB_9H_{10}]



M 240.3 (ion)
Paramagnetic.

Me_4N salt: [62580-70-5].
Violet needles (MeOH).

Dolansky, J. *et al*, *Chem. Ind.* (*London*), 1976, 853 (*synth, nmr*)
Subrtova, V. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 2720 (*struct*)

$C_6H_{15}Ca_3O_{46}Si_8Y_4$ IC-005218

Caysichite, 9CI

[52932-28-2]

$(Ca_3Ln)Y_4[Si_8O_{20}][CO_3]_6(OH).7H_2O$

M 1523.6
Rare mineral with a double crankshaft chain struct. A rare earth silicate. Also formulated as $\frac{1}{3}(Ca,Gd)_2(Si,Al)_4O_{10}(CO_3)_3.4H_2O$. Occurs in granite pegmatite in Quebec. Also in amazonitic pectolites in Kola Peninsula, USSR. Colourless to white, more rarely yellow or green orthorhombic encrustations and stalactites. Effervesces slowly in cold, dil. HCl.

Mellini, M. *et al*, *Can. Mineral.*, 1978, **16**, 81 (*cryst struct*)
Hogarth, D.D. *et al*, *Can. Mineral.*, 1974, **12**, 293 (*mineral*)
Voloshin, A.V. *et al*, *Mineral. Zh.*, 1986, **8**, 90; *CA*, **105**, 156236d (*occur*)

$C_6H_{15}ClHfO_3$ IC-005219

Chlorotriethoxyhafnium(*IV*), 11CI

[101803-59-2]

$(EtO)_3HfCl$ (C_{3v})

M 349.1
Synth. from $Hf(OEt)_4$ and MeCOCl in boiling C_6H_6. A convenient source of $(EtO)_3Hf$ alkyls by reaction with LiR.

Kauffmann, T. *et al*, *Tetrahedron Lett.*, 1985, **26**, 4059 (*synth*)

$C_6H_{15}ClO_3Ti$ IC-005220

Chlorotriethoxytitanium(*IV*), 11CI

[3712-48-9]

$TiCl(OEt)_3$

M 218.5
Trimeric in C_6H_6 and dimeric in dioxan. Synth. from $TiCl_4$ + $3Ti(OEt)_4$ in C_6H_6 and purifying by vacuum distillation, or from $Ti(OEt)_4$ with AcCl. Used to catalyse ethylene polym. and acrylonitrile/cycloolefin polym. Pale yellow liq. Bp_{18} 176°.

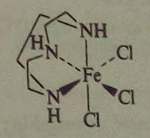
Cullinane, N.M. *et al*, *J. Appl. Chem.*, 1952, **2**, 250 (*synth*)
Felz, A., *Z. Anorg. Allg. Chem.*, 1964, **334**, 186 (*synth*)
Weingarten, H. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 724 (*pmr*)
Furukawa, J. *et al*, *Polym. J.* (*Tokyo*), 1983, **15**, 435; *CA*, **100**, 34862f (*use*)
U.S. Pat., 4 518 751, (1985); *CA*, **103**, 71824c (*use*)

$C_6H_{15}Cl_3FeN_3$ IC-005221

Trichloro(1,4,7-triazacyclononane)iron(*III*)

Trichloro(octahydro-1H-1,4,7-triazonine-N^1,N^4,N^7)iron(III), *11CI*

[86823-88-3]



M 291.4
Synth. from $FeCl_3.6H_2O$ + 1,4,7-triazacyclononane. Precursor to dinuclear complexes used as model for proteins such as hemerthyrin. Air-stable bright yellow cryst. Insol. EtOH.

N,N′,N″-Tri-Me: see *Trichloro(1,4,7-trimethyl-1,4,7-triazacyclononane)iron*(III), *IC-006570*

Wieghardt, K. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 727 (*synth, use*)

$C_6H_{15}Cl_3NO_2Ti$ IC-005222

(Acetonitrile)trichlorobis(ethanol)titanium(*III*)

Titanium(III) chloride acetonitrile bis(ethanol)

[87052-12-8]

$(H_3CCN)TiCl_3(EtOH)_2$

M 287.4

Octahedral, config. not reported. Synth. from $TiCl_3$·3MeCN + EtOH.

Kobutova, M. *et al*, *Proc. Conf. Coord. Chem.*, 9th, 1983, 169; *CA*, **99**, 114906z (*synth, ir, thermal anal*)

$C_6H_{15}Cl_3PPt^{\ominus}$ IC-005223

Trichloro(triethylphosphine)platinate(*II*)(1−), 11Cl

[44968-43-6]

$[PtCl_3(PEt_3)]^{\ominus}$

M 419.5 (ion)

Adds Cl_2 to afford $[Pt(PEt_3)Cl_5]^{\ominus}$.

Et_4N salt: [56544-60-6].

Yellow cryst. (CH_2Cl_2/Me_2CO). Sol. CH_2Cl_2.

Tetrapropylammonium salt: [19508-37-3].

Yellow cryst. Sol. CH_2Cl_2. Mp 195°.

Et_3PPh salt: [51414-76-7].

Yellow solid (C_6H_6/EtOAc). Sol. $CHCl_3$. Mp 123.9-124.9°

Duddell, D.A. *et al*, *J. Chem. Soc. A*, 1970, 545 (*synth, raman, ir*)
Mather, G.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2095 (*synth, nmr*)
Coulson, D.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2459 (*synth, pmr, reaction*)
Bushnell, G.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 572 (*synth, cryst struct*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 459 (*nmr*)
Gosling, R. *et al*, *Inorg. Chem.*, 1983, **22**, 1235 (*reaction*)
Phillips, J.R. *et al*, *Inorg. Chem.*, 1986, **25**, 1503 (*uv-vis*)

$C_6H_{15}Cl_4PTi$ IC-005224

Tetrachloro(triethylphosphine)titanium(*IV*), 11Cl

Titanium(IV) chloride triethylphosphine

[101050-07-1]

Et_3PTiCl_4

M 307.8

Synth. by adding excess $TiCl_4$ in CH_2Cl_2 to Et_3P in CH_2Cl_2. Dark red solid.

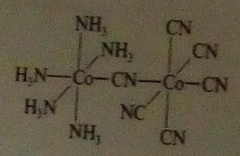
Calderazzo, F. *et al*, *Helv. Chim. Acta*, 1971, **54**, 1156 (*synth*)
Gordon, D. *et al*, *Inorg. Chim. Acta*, 1986, **111**, 77 (*P-31 nmr*)

$C_6H_{15}Co_2N_{11}$ IC-005225

Pentaammine(μ-cyano-*C*:*N*)pentakis(cyano-*C*)dicobalt(*III*), 8Cl

Pentaamminecobalt(III)-μ-*isocyanopentacyanocobaltate*(III)

[22653-93-6]



M 359.1

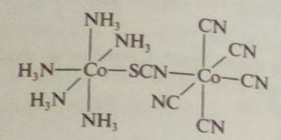
Ir suggests cyanide bridge in binuclear struct. Yellow solid.

Castello, R.A. *et al*, *Inorg. Chem.*, 1971, **10**, 203 (*synth, uv, ir*)

$C_6H_{15}Co_2N_{11}S$ IC-005226

Pentaamminepentakis(cyano-*C*)[μ-(thiocyanato-*N*:*S*)]dicobalt(*III*), 9Cl

Pentaamminecobalt(III)-μ-*thiocyanato*(*pentacyano*)*cobalt*(III)



$Co(NH_3)_5SCN$-*form*

M 391.1

$Co(NH_3)_5SCN$-form [38893-10-6]

Synth. from $K_2[Co(CN)_5H_2O]$ + $[Co(NH_3)_5SCN](ClO_4)_2$ in H_2O at 0°. Pale pink solid + $1H_2O$. Sol. H_2O; insol. most org. solvs.

$Co(NH_3)_5NCS$-form [38893-09-3]

Synth. from $[Co(CN)_5H_2O]^{2\ominus}$ + $[Co(NH_3)_5NCS]^{2\oplus}$ in H_2O with a little $HClO_4$ at 50°, followed by ion exchange. Orange solid + $1H_2O$.

[55493-58-8]

Buckley, R.C. *et al*, *Inorg. Chem.*, 1972, **11**, 1723 (*synth, uv, ir*)

$C_6H_{15}Cr_2N_{11}S_6$ IC-005227

Pentaammine[μ-(thiocyanato-*N*:*S*)]pentakis(thiocyanato-*N*)dichromium(*III*), 9Cl

μ-Thiocyanatopentaamminechromium(III) *pentaisothiocyanatochromium*(III)

[37766-08-8]

$(H_3N)_5Cr{-}SCN{-}Cr(NCS)_5$

M 537.6

Struct. proposed on basis of ir. Rel. light- and heat-stable solid + $3H_2O$. Prac. insol. H_2O; dec. in MeCN, DMF.

Buckley, R.C. *et al*, *Inorg. Chem.*, 1972, **11**, 1723 (*synth, ir*)

$C_6H_{15}CuIO_3P$ IC-005228

Iodo(triethyl phosphite-*P*)copper(*I*), 9Cl

[51717-23-8]

$ICuP(OEt)_3$

M 356.6

Probably tetrameric in solid state.

Tetramer(?):

$C_{24}H_{60}Cu_4I_4O_{12}P_4$ M 1426.4

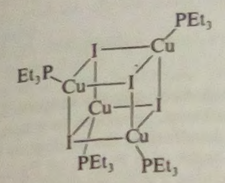
Reagent for Ullmann coupling of *o*-haloarylimines. Cryst. (C_6H_6). Sol. C_6H_6. Mp 110-111°.

Nishizawa, Y., *Bull. Chem. Soc. Jpn.*, 1961, **34**, 1170 (*synth*)
Sato, T. *et al*, *Tetrahedron Lett.*, 1973, 4221 (*use*)
Ziegler, F.E. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 8282 (*use*)
Maryanoff, B.E. *et al*, *J. Org. Chem.*, 1979, **44**, 4410 (*use*)

$C_6H_{15}CuIP$ IC-005229

Iodo(triethylphosphine)copper(*I*), 9Cl

[56667-47-1]



M 308.6

Tetrameric.

Tetramer: [51364-98-8]. *Tetra-μ$_3$-iodotetrakis(triethylphosphine)tetracopper*

$C_{24}H_{60}Cu_4I_4P_4$ M 1234.4

Solid state struct. based on Cu_4I_4 cube with Cu—Cu 292.7 pm. Colourless cryst. (C_6H_6). Spar. sol. C_6H_6; insol. EtOH, Me_2CO. Mp 236-240° (softens at 230°).

Mann, F.G. *et al*, *J. Chem. Soc.*, 1936, 1503 (*synth*)
Churchill, M.R. *et al*, *Inorg. Chem.*, 1974, **13**, 1899 (*cryst struct*)
Bowmaker, G.A. *et al*, *Aust. J. Chem.*, 1978, **31**, 2137 (*ir, raman*)
Valigura, D. *et al*, *Bull. Soc. Chim. Belg.*, 1980, **89**, 831 (*nqr*)

$C_6H_{15}ErO_9S_3$ IC-005230

Erbium(*III*) ethylsulfate

$Er[OS(O)_2Et]_3$

M 494.6

Obt. as nonahydrate.

Nonahydrate: [56422-26-5]. *Nonaaquaerbium(3+) tris(ethylsulfate)*

Pink cryst. Sol. H_2O. Contains $[Er(OH_2)_9]^{3\oplus}$ ions (tricapped trigonal prismatic).

Fitzwaltez, D.R. *et al*, *Z. Kristallogr.*, 1959, **112**, 362 (*synth, cryst struct*)
Cooke, A.H. *et al*, *Proc. Phys. Soc., London*, 1965, **85**, 767 (*magnetism*)
Hill, J.L. *et al*, *Phys. Rev.*, 1966, 152, 482 (*ir*)
Staveley, L.A.K. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
Schaack, G. *et al*, *Can. J. Chem.*, 1973, **53**, 1023 (*raman*)
Albertsson, J. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1460 (*synth, struct*)
Kato, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 589 (*uv-vis, mcd*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1981, **C8**, 362 (*rev*)

$C_6H_{15}FeO_3$ IC-005231

Iron(*III*) ethoxide

Ferric ethoxide. Triethoxyiron(III). *Ethanol iron(3+) salt (3:1)*

$Fe(OEt)_3$

M 191.0

Trimeric struct. proposed. Synth. from $FeCl_3$ + EtOH + NH_3. Brown cryst. (EtOH). Sol. C_6H_6. Magnetic behaviour supports cluster formn. Antiferromagnetic coupling of $S = \frac{5}{2}$ Fe centres obsd.

Trimer:

$C_{18}H_{45}Fe_3O_9$ M 573.0

Bradley, D.C. *et al*, *J. Chem. Soc.*, 1958, 126 (*synth*)
Adams, R.W. *et al*, *Inorg. Chem.*, 1966, **5**, 346 (*magnetism*)

$C_6H_{15}GaO_3$ IC-005232

Gallium(*III*) ethoxide

Triethoxygallium

$Ga(OEt)_3$

M 204.9

Tetrameric in C_6H_6. Synth. from $GaCl_3$ and NaOEt in EtOH. Colourless v. moisture sensitive needles (EtOH). Sol. C_6H_6; sl. sol. hexane. Mp 144.5°. $Subl._{0.5}$ 180-190°. Reacts with wide range of ROH to give $Ga(OR)_3$.

Reinmann, R. *et al*, *Z. Naturforsch., B*, 1965, **20**, 524 (*synth*)
Bindal, S.R. *et al*, *J. Chem. Soc. A*, 1969, 863 (*synth, props, ir*)

$C_6H_{15}GdO_9S_3$ IC-005233

Gadolinium(*III*) ethylsulfate

$Gd[OS(O)_2Et]_3$

M 484.6

Obt. as nonahydrate.

Nonahydrate: [59922-12-2]. *Nonaaquagadolinium(3+) tris(ethylsulfate)*

Colourless cryst. Sol. H_2O. Contains $[Gd(H_2O)_8]^{3\oplus}$ ions (tricapped trigonal prisms).

Van der Broek, J. *et al*, *Physica* (*Amsterdam*), 1963, **29**, 948 (*magnetism*)
Staveley, L.A.K. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
Albertsson, J. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1640 (*synth, struct*)
Gerkin, R.E. *et al*, *J. Chem. Phys.*, 1977, **66**, 4166 (*esr*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. Vol.*, 1987, **C8**, 362 (*rev*)

$C_6H_{15}HoO_9S_3$ IC-005234

Holmium(*III*) ethylsulfate

Tris(ethanesulfonato)holmium

$Ho(OSO_2Et)_3$

M 492.3

Nonahydrate: [55664-38-5]. *Nonaaquaholmium(3+) tris(ethanesulfonate)*

$C_6H_{33}HoO_{18}S_3$ M 654.4

Pale yellow cyrst. Sol. H_2O. Contains tricapped prismatic $[Ho(H_2O)_8]^{3\oplus}$.

Fitzwater, D.R. *et al*, *Z. Kristallogr.*, 1959, **112**, 362 (*cryst struct*)
Coohe, A.H. *et al*, *Proc. Phys. Soc., London*, 1965, **85**, 767 (*magnetism*)
Staveley, L.A.K. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
Shaack, G. *et al*, *Can. J. Chem.*, 1973, **51**, 1023 (*raman*)
Hubbard, C.R. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 2613 (*cryst struct*)
Albertsson, J. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1460 (*synth, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, *Suppl. vol.*, 1981, **C8**, 362 (*rev*)

$C_6H_{15}InS_3$ IC-005235

Tris(ethanethiolato)indium

Tris(ethylmercapto)indium

$In(SEt)_3$

M 298.2

Monomeric. Air- and moisture sensitive colourless solid (CH_2Cl_2). Sol. CH_2Cl_2. Mp 257°.

Hoffmann, G., *J. Organomet. Chem.*, 1988, **338**, 305 (*synth, pmr, ir*)

$C_6H_{15}LaO_9S_3$ IC-005236

Lanthanum(*III*) ethylsulfate

Tris(ethanesulfonato)lanthanum(III)

$La(OSO_2Et)_3$

M 466.2

Nonahydrate: [59922-21-3]. *Nonaaqualanthanum(3+) tris(ethanesulfonate)*

$C_6H_{33}LaO_{18}S_3$ M 628.4

Similar struct. for other lanthanides, forming an isomorphous series. Colourless cryst. Sol. H_2O. Tricapped trigonal prismatic $La(OH_2)_9^{3\oplus}$ ions present. Diamagnetic.

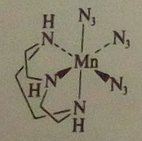
Ketelaar, J.A.A., *Physica (Amsterdam)*, 1937, **8**, 619 (*cryst struct*)
Geserich, M.P. *et al*, *Z. Naturforsch., A*, 1965, **20**, 289 (*ir, raman*)
Staveley, L.A.K. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
Albertsson, J. *et al*, *Acta Crystallogr., Sect. B*, 1972, **33**, 1460 (*cryst struct*)
Kato, Y. *et al*, *Spectrochim. Acta, Part A*, 1977, **33**, 1033 (*ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. vol., 1981, **C8**, 362 (*rev*)
Gerkin, R.E. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 781.

$C_6H_{15}MnN_{12}$ IC-005237

Tris(azido)(1,4,7-triazacyclononane-*N,N',N''*) manganese(*III*)

Triazido(octahydro-1H-1,4,7-triazonine-N^1,N^4,N^7*) manganese*(III), *12CI*

[107760-70-3]



M 310.2

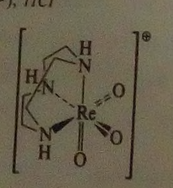
Octahedral at Mn. Synth. from $Mn_2(\mu\text{—}O)(\mu\text{—}OAc)_2L_2$ and NaN_3 in EtOH. Red brown cryst. (MeCN). Insol. H_2O. $\mu_{eff} = 4.96\mu_B$.

Wieghardt, K. *et al*, *Inorg. Chim. Acta*, 1987, **126**, 39 (*synth, cryst struct, magnetism*)

$C_6H_{15}N_3O_3Re^{\oplus}$ IC-005238

Trioxo(1,4,7-triazacyclononane-*N,N',N''*)rhenium(*VII*) (1+)

(Octahydro-1H-1,4,7-triazonine-N^1,N^4,N^7*) trioxorhenium(1+), 11CI*



M 363.4 (ion)

Distorted octahedral at Re.

Chloride: [101566-56-7].

Synth. from $[(C_6H_{15}N_3)Re(NO)(CO)_2](BF_4)_2$ and H_2O_2, followed by NaCl aq. Colourless cryst. (H_2O).

Wieghardt, K. *et al*, *Inorg. Chem.*, 1986, **25**, 1659 (*synth, ir, cryst struct*)

$C_6H_{15}O_3P$ IC-005239

Triethyl phosphite, 9CI, 8CI

Triethoxophosphorus(III)

[122-52-1]

$(EtO)_3P$

M 166.1

Widely used organophosphorus reagent. Deoxygenates epoxides to alkenes, peroxides to ethers, hydroperoxides to alcohols, desulfurizes the analogous sulfur compds. Condensing agent with Py/Br_2 or Py/I_2 for synth. of esters and amides. Deoxygenates *tert*-amine *N*-oxides. Deoxygenates aryl nitro groups via nitrenes giving syntheses of heterocyclic compds. including phenazines, phenoxazines, phenothiazines, indazoles, triazoles and also azepines. Converts aromatic dicarbonyl compds. to epoxides. Carbonyl compds. may be reductively dimerised, e.g. phthalic anhydride → biphthalyl. Widely used in Arbuzov reactions for synth. of phosphonic and phosphinic di-Et-esters, for use in Wadsworth-Emmons reactions. Liq. with characteristic, obnoxious, phosphite odour. d_4^{20} 0.963. Bp_{16} 57-58°. n_D^{25} 1.4105.

▷ TH1130000.

Halman, M., *J. Chem. Soc.*, 1963, 2853 (*uv*)
Gerken, T.A. *et al*, *J. Magn. Reson.*, 1976, **24**, 155 (*pmr, cmr, P-31 nmr*)
Labintsev, V.B. *et al*, *Zh. Org. Khim.*, 1977, **13**, 1141; *J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 1050 (*ms*)
Cadogan, J.I.G., *Organophosphorus Reagents in Org. Synth.*, Ed., Academic Press, 1979 (*uses*)
Chattopadhyay, S. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1981, **24**, 27 (*pe*)
Vasil'ev, V.V. *et al*, *Zh. Obshch. Khim.*, 1981, **51**, 2134; *J. Gen. Chem. USSR (Engl. Transl.)*, 1981, **51**, 1836 (*O-17 nmr*)
Cload, A. *et al*, *Org. Mass Spectrom.*, 1983, **18**, 57 (*ms*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3354.

$C_6H_{15}O_3PS$ IC-005240

***O,O,O*-Triethyl phosphorothioate, 9CI**

O,O,O-*Triethyl thiophosphate. Triethoxothiophosphorus*(V)

[126-68-1]

$(EtO)_3P{=}S$

M 198.2

Liq. d_0^{20} 1.076. Bp_8 88-89°. n_D^{20} 1.4488. Isom. to *O,O,S*-Triethyl phosphorothioate, IC-005241 when heated.

▷ Highly toxic. TG3675000.

McIvor, R.A. *et al*, *Can. J. Chem.*, 1950, **36**, 820 (*ir*)
Cadogan, J.I.G. *et al*, *J. Chem. Soc.*, 1961, 3067, 5524 (*synth*)
Zemlyanskii, N.I. *et al*, *Zh. Obshch. Khim.*, 1961, **30**, 4056; *J. Gen. Chem. USSR (Engl. Transl.)*, 1961, **30**, 4018 (*raman*)
Williamson, M.P. *et al*, *J. Phys. Chem.*, 1968, **72**, 4043 (*pmr*)
Zwierzak, A., *Tetrahedron*, 1969, **25**, 5177 (*synth*)
Nifant'ev, E.E. *et al*, *Zh. Obshch. Khim.*, 1975, **45**, 295; *J. Gen. Chem. USSR (Engl. Transl.)*, 1975, **45**, 282 (*synth*)
Gurley, T.W. *et al*, *Anal. Chem.*, 1976, **48**, 1137 (*P-31 nmr*)
Buckland, S.J. *et al*, *J. Photochem.*, 1987, **36**, 39 (*reaction*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3355.

$C_6H_{15}O_3PS$ IC-005241

***O,O,S*-Triethyl phosphorothioate, 9CI, 8CI**

O,O,S-*Triethyl thiophosphate*

[1186-09-0]

$(EtO)_2P(O)SEt$

M 198.2

Liq. d_4^{20} 1.11. Bp_3 83-85°. n_D^{20} 1.4590.

▷ High oral toxicity. TG3700000.

McIvor, R.A. *et al*, *Can. J. Chem.*, 1958, **36**, 820 (*ir*)
Mastryukova, T.A. *et al*, *Zh. Obshch. Khim.*, (*Engl. transl.* p. 92), 1964, **34**, 94 (*synth*)
Zimin, M.G. *et al*, *Zh. Obshch. Khim.*, (*Engl. transl.* p. 1922), 1972, **49**, 2189 (*synth, P nmr*)
Mallipudi, N.M. *et al*, *J. Agric. Food Chem.*, 1979, **27**, 463 (*tox*)
Verschoyle, R.D. *et al*, *Arch. Toxicol.*, 1982, **51**, 221 (*tox*)

$C_6H_{15}O_3PSe$ IC-005242

***O,O,O*-Triethyl phosphoroselenoate, 9CI, 8CI**

Triethyl selenophosphate. Triethoxoselenidophosphorus(V)

[2651-89-0]

$(EtO)_3P{=}Se$

M 245.1

Liq. d_4^{20} 1.304. Bp_{20} 117°, Bp_9 85°. n_D^{20} 1.4730. Fire-proofer for lubricating oils.

Nuretdinov, I.A. *et al*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1968, 2831; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 2685 (*synth, ir*)
Kainosho, M., *J. Phys. Chem.*, 1970, **74**, 2853 (*pmr*)
Stec, W.J. *et al*, *Phosphorus*, 1972, **2**, 97 (*P-31 nmr*)
Shagidullin, R.R. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 184; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1976, 174 (*uv*)
Glidewell, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 527 (*ir, P-31 nmr*)
Turkevich, V.V. *et al*, *Zh. Obshch. Khim.*, 1977, **47**, 2388; *J. Gen. Chem. USSR (Engl. Transl.)*, 1977, **47**, 2181 (*ir*)
Ando, F. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 807 (*ir, pmr*)
Zverev, V.V. *et al*, *Zh. Obshch. Khim.*, 1981, **51**, 303; *J. Gen. Chem. USSR (Engl. Transl.)*, 1981, **51**, 242 (*pe*)

$C_6H_{15}O_3Sb$ IC-005243

Triethyl antimonite

Triethoxystibine. Antimonic acid, (H_3SbO_3), triethyl ester, 9CI, 8CI. Triethoxoantimony

[10433-06-4]

$Sb(OEt)_3$

M 256.9

Liq. Bp_{30} 118°, $Bp_{0.5}$ 71-73°, $Bp_{0.05}$ 37-38°. n_D^{20} 1.4945.

Kiennemann, A. *et al*, *J. Organomet. Chem.*, 1972, **35**, 143 (*synth*)
Brill, T.B. *et al*, *Inorg. Chem.*, 1973, **12**, 1884 (*synth, ir, raman*)
Bowen, L.H. *et al*, *Inorg. Chem.*, 1974, **13**, 1787 (*mössbauer*)
Krommes, P. *et al*, *J. Organomet. Chem.*, 1975, **97**, 59 (*synth*)

$C_6H_{15}O_4P$ IC-005244

Triethyl phosphate, 9CI

Triethoxooxophosphorus(V)

[78-40-0]

$(EtO)_3P{=}O$

M 182.1

Ethylating agent for nitrogen heterocyclic compds. Pleasant smelling liq. Misc. H_2O. d_4^{25} 1.06. Bp 215°, Bp_{50} 128°, Bp_5 75°. n_D^{20} 1.4053.

▷ TC7900000.

[66642-65-7, 114019-85-1]

Evans, D.P. *et al*, *J. Chem. Soc.*, 1930, 1310 (*synth*)
Cox, J.R. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 5441 (*synth*)
Mitsunobu, O. *et al*, *Bull. Chem. Soc. Jpn.*, 1961, **40**, 935 (*synth*)
Hata, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1962, **35**, 1106 (*synth*)
Mukaiyama, T. *et al*, *J. Org. Chem.*, 1962, **27**, 1815; 1963, **28**, 481 (*synth*)
Crofts, P.C. *et al*, *J. Chem. Soc.*, 1963, 2559 (*synth*)
Strukov, O.G. *et al*, *Zh. Prikl. Spektrosk.*, 1967, **7**, 209; *J. Appl. Spectrosc. USSR (Engl. Transl.)*, 1967, **7**, 150 (*ir*)
Betteridge, D. *et al*, *Anal. Chem.*, 1972, **44**, 2005 (*pe*)
Gerken, T.A. *et al*, *J. Magn. Reson.*, 1976, **24**, 155 (*pmr*)
Kawazoe, Y. *et al*, *Chem. Pharm. Bull.*, 1982, **30**, 2077 (*props, use*)
Cload, P.A. *et al*, *Org. Mass Spectrom.*, 1983, **18**, 57 (*ms*)
Appling, J.R. *et al*, *Org. Mass Spectrom.*, 1985, **20**, 343 (*ms*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3354.

$C_6H_{15}O_4V$ IC-005245

Triethoxyoxovanadium(*V*), 11CI

Vanadic acid triethyl ester, 9CI

[1686-22-2]

$VO(OEt)_3$

M 202.1

Tetrahedral (C_{3v}). Synth. from $VOCl_3$ and EtOH in the presence of NH_3. Used in vapour phase epitaxial formation of field effect transistors. Colourless, moisture-sensitive liq. $Bp_{0.1}$ 67°.

Gervaise, D. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 3679 (*synth, magnetism*)
Buslaev, Yu.A. *et al*, *Koord. Khim.*, 1977, **3**, 216; *CA*, **86**, 182199c (*synth*)
Adler, B. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **431**, 227 (*ms, props*)
Aizutullova, R.M. *et al*, *Zh. Fiz. Khim.*, 1983, **57**, 443 (*thermochem*)
Japan. Pat., 59 169 123, (1984); *CA*, **102**, 124032f (*use*)

$C_6H_{15}O_9PrS_3$ IC-005246

Praseodymium(*III*) ethylsulfate

$Pr[OS(O)_2Et]_3$

M 468.2

Nonahydrate: [56487-88-8]. *Nonaaquapraseodymium(3+) tris(ethylsulfate)*

Green cryst. Sol. H_2O. Contains $Pr(OH_2)_9^{3\oplus}$ ions (tricapped trigonal prism).

Ketelaar, J.A.A., *Physica (Amsterdam)*, 1937, **8**, 619.
Fitzwater, D.R. *et al*, *Z. Kristallogr.*, 1959, **112**, 362.
Hellwege, K.H. *et al*, *Z. Phys.*, 1962, **167**, 477 (*magnetism*)
Albertsson, J. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1460 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. Vol., 1981, **C8**, 362 (*rev*)
Gerkin, R.E. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 781 (*cryst struct*)

$C_6H_{15}O_9S_3Y$ IC-005247

Yttrium(*III*) ethylsulfate

$Y[OS(O)_2Et]_3$

M 416.2

Nonahydrate: [56422-22-1]. *Nonaaquayttrium(3+) tris(ethylsulfate)*

When subst. by Yb, substantial proton polarization obtained; applications in nuclear + high energy expts. Colourless cryst. Sol. H_2O. Contains tricapped trigonal prismatic $Y(OH_2)_9^{3\oplus}$ ions.

Button-Shafer, J. *et al*, *Phys. Rev. Lett.*, 1977, **39**, 677 (*use*)
Broach, R.W. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2317 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, Suppl. Vol., 1981, **C8**, 362 (*rev*)
Gerkin, R.E. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 781 (*cryst struct*)

$_{15}O_9S_3Yb$ IC-005248

terbium(*III*) ethylsulfate

$Yb[OS(O)_2Et]_3$

500.4
t. as nonahydrate.
nahydrate: [56422-18-5]. *Nonaaquaytterbium(3+) ris(ethylsulfate)*
Colourless cryst. Sol. H_2O. Contains $[Yb(OH_2)_8]^{3\oplus}$ ions tricapped trigonal prismatic).
ske, A.H. *et al, Philos. Mag.*, 1957, **2**, 928 (*magnetism*)
veley, L.A.K. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 231 (*synth*)
erisson, J. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 1460 (*synth, cryst struct*)
elln Handbook Inorg. Chem., Syst. No. 39, Suppl., 1981, **C8**, 362 (*rev*)

$_6PS_3$ IC-005249

ethyl phosphorotrithioite, 9CI

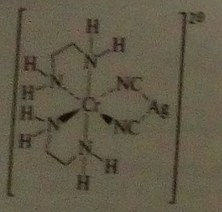
ethyl trithiophosphite. Tri(ethylthio)phosphorus(III)
8-62-0]

$(EtS)_3P$

214.3
and for Hg and Au. Liq. d_4^{25} 1.16. Mp −32°. Bp_{18} 140-43°.
5700000.
del: Tri(ethylthio)methylphosphonium iodide
$_7H_{18}IPS_3$ M 356.2
Solid. Mp 191°.
del: Ethyltri(ethylthio)phosphonium iodide
$_8H_{20}IPS_3$ M 370.3
Solid. Mp 125-127°.
pert, A. *et al, J. Am. Chem. Soc.*, 1938, **60**, 2370 (*synth, deriv*)
rnova, A.V. *et al, Zh. Obshch. Khim.*, 1979, **49**, 2002; *J. Gen. Chem. USSR (Engl. Transl.)*, 1979, **49**, 1760 (*ir, struct*)
tin, V.P. *et al, Zh. Obshch. Khim.*, 1982, **52**, 498, 2698; *J. Gen. Chem. USSR (Engl. Transl.)*, 1982, **52**, 437, 2379 (*synth, P-31 nmr*)
rov, V.V. *et al, Zh. Obshch. Khim.*, 1983, **53**, 1968; *J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 1775 (*pe*)
ant'ev, E.E. *et al, Zh. Obshch. Khim.*, 1983, **53**, 2695; *J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 2429 (*synth, P-31 nmr*)
rgova, E.A. *et al, Zh. Prikl. Spektrosk.*, 1987, **46**, 761; *J. Appl. Spectrosc. USSR (Engl. Transl.)*, 1987, **46**, 467 (*ir, raman*)

$_6AgCrN_8^{2\oplus}$ IC-005250

(cyano-*N*)bis(1,2-ethanediamine-*N,N'*)erchromium(2+)



332.0 (ion)
m
inkage isomer of *cis*-$[Cr(CN)_2(en)_2]^{\oplus}$ formed through nteraction with $Ag^{\oplus}$ (see also Bis[dicyanosilver(*I*)-*N*] ris(ethylenediamine)chromium(*III*), IC-006053). recipitation of AgI regenerates uv spectrum of *cis*-$Cr(CN)_2(en)_2]^{\oplus}$.
erchlorate: [75047-20-0].

Synth. from $AgNO_3$ and *cis*-$[Cr(CN)_2(en)_2]ClO_4$ followed by $NaClO_4$. Yellow orange solid.
Heatherington, A. *et al, Inorg. Chim. Acta*, 1980, **44**, L279 (*synth, uv, ir*)

$C_6H_{16}AlNaO_4$ IC-005251

Sodium dihydrobis(2-methoxyethanolato-*O,O'*)aluminate(1−)

Sodium bis(2-methoxyethoxy)aluminium hydride. RED-Al. SDMA. Vitride. Synhydride
[22722-98-1]

$NaAlH_2(OCH_2CH_2OMe)_2$

M 202.1
Oligomeric structs. proposed in soln. Widely used as reducing agent in org. chem. Viscous moisture sensitive liq. Used as 70% soln. in toluene. Sol. hydrocarbons, ethers. ΔH_f −1316 kJ mol^{-1}.
Walker, E.R.H., *Chem. Soc. Rev.*, 1976, **5**, 23 (*use*)
Inorg. Synth., 1978, **18**, 149 (*synth*)
Štrouf, O. *et al, J. Organomet. Chem. Libr.*, 1985, **150** (*rev, props, use*)
Heřmánek, S. *et al, Z. Naturforsch., B*, 1985, **40**, 582 (*Al-27 nmr*)
Vit, J., *HEXCEL Corporation Technical Information Bull.*, 1986 (*rev, use*)

$C_6H_{16}AlO_2^{\ominus}$ IC-005252

Dihydrodiisopropoxyaluminate(1−)

Dihydrobis(2-propanolato)aluminate(1−)

$[AlH_2[OCH(CH_3)_2]_2]^{\ominus}$

M 147.1 (ion)
Detected in soln. by nmr as Me_4N salt.
Li salt: [70556-31-9].
Shown to be a mixt. of $LiAlH_4$ and $LiAl[OCH(CH_3)_2]_4$.
Turova, N.Ya. *et al, Zh. Obshch. Khim.*, 1977, **47**, 1338; *Inorg. Chim. Acta*, 1977, **21**, 157 (*synth, powder struct*)
Heřmánek, S. *et al, Z. Naturforsch., B*, 1987, **42**, 539 (*Al-27 nmr*)

$C_6H_{16}AlO_3^{\ominus}$ IC-005253

Triethoxyhydroaluminate(1−)

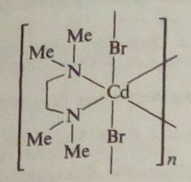
$[AlH(OEt)_3]^{\ominus}$

M 163.1 (ion)
Li salt: [17250-30-5].
Synth. from $LiAlH_4$ and 3EtOH in Et_2O. Selective reducing agent. White moisture-sensitive solid. May be assoc. in soln.
Brown, H.C. *et al, J. Am. Chem. Soc.*, 1964, **86**, 1089 (*synth, use*)
Haubenstock, H., *J. Org. Chem.*, 1973, **38**, 1765 (*use*)
Peretti, D. *et al, Bull. Soc. Chim. Fr.*, 1974, 2925 (*use*)
Turova, N.Ya., *Inorg. Chim. Acta*, 1977, **21**, 157 (*synth, powder struct*)
Turova, N.Ya. *et al, Zh. Obshch. Khim.*, 1977, **47**, 1338 (*props, powder struct*)
Gavrilenko, V.V. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1979, **28**, 1273 (*Al-27 nmr*)
Gless, R.D. *et al, J. Org. Chem.*, 1979, **44**, 1324 (*use*)
Hermanek, S. *et al, Z. Naturforsch., B*, 1987, **42**, 539 (*ir*)

$C_6H_{16}Br_2CdN_2$ IC-005254

Dibromo(*N,N,N',N'*-tetramethylethylenediamine)cadmium

(Tetramethylethylenediamine)cadmium dibromide
[28377-04-0]

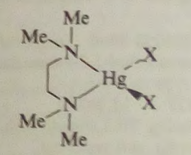


M 388.4
Polymeric in solid state with octahedral Cd. Plates (MeOH). Mp 245-247°.
[26758-69-0]
Abraham, M.H. *et al, Can. J. Chem.*, 1970, **48**, 181 (*ir, raman*)
Bell, N.A. *et al, Thermochim. Acta*, 1973, **6**, 275 (*synth, thermal anal*)
Htoon, S. *et al, J. Cryst. Mol. Struct.*, 1974, **4**, 97; 1976, **6**, 55 (*cryst struct*)

$C_6H_{16}Br_2HgN_2$ IC-005255

Dibromo(*N,N,N',N'*-tetramethylethylenediamine)mercury

Dibromo(N,N,N',N'-tetramethyl-1,2-ethanediamine-N,N')mercury
[49662-44-4]



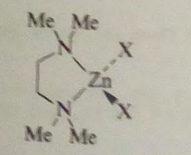
X = Br

M 476.6
Needles (MeOH). Mp 164°, Mp 145°.
[61944-77-2]
Abraham, M.H. *et al, Can. J. Chem.*, 1970, **48**, 181 (*synth, ir, raman*)
Bell, N.A. *et al, Thermochim. Acta*, 1973, **6**, 275 (*thermal anal*)
Htoon, S. *et al, J. Cryst. Mol. Struct.*, 1976, **6**, 55 (*cryst struct*)
Bryukhova, E.V. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1977, **22**, 1846 (*nqr*)

$C_8H_{20}Br_2N_2Zn$ IC-005256

Dibromo(*N,N,N',N'*-tetramethylethylenediamine)zinc

(Tetramethylethylenediamine)zinc dibromide
[28307-98-4]



X = Br

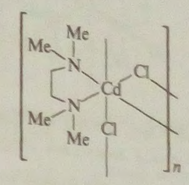
M 341.4
Plates (EtOH). Mp 182°.
Coates, G.E. *et al, J. Chem. Soc.*, 1964, 166 (*synth, ir*)
Nottes, J.G. *et al, J. Organomet. Chem.*, 1964, **1**, 377 (*synth*)

Abraham, M.H. *et al, Can. J. Chem.*, 1970, **48**, 181 (*synth, ir, raman*)
Bell, N.A. *et al, Thermochim. Acta*, 1973, **6**, 275 (*thermal anal*)
Htoon, S. *et al, J. Cryst. Mol. Struct.*, 1976, **6**, 55 (*cryst struct*)

$C_6H_{16}CdCl_2N_2$ IC-005257

Dichloro(*N,N,N',N'*-tetramethylethylenediamine)cadmium

Dichloro(N,N,N',N'-tetramethyl-1,2-ethanediamine-N,N')cadmium. (Tetramethylethylenediamine)cadmium dichloride
[27816-63-3]



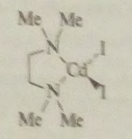
Solid state struct.

M 299.5
Octahedral in solid state with *cis*-chloride bridge. Air-stable colourless needles (EtOH or MeOH). Sl. sol. hot EtOH, hot Me_2CO. Mp 250° dec. Dec. in hot H_2O to $Cd(OH)_2$. Loses TMED on heating to give $CdCl_2$·(TMED).
[61896-89-7]
Mann, F.G. *et al, J. Chem. Soc.*, 1958, 2772 (*synth*)
Coates, G.E. *et al, J. Chem. Soc.*, 1964, 166 (*ir*)
Abraham, M.H. *et al, Can. J. Chem.*, 1970, **48**, 181 (*synth, ir, raman*)
Caulton, K.G., *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 533 (*synth, pmr, ms*)
Bell, N.A. *et al, Thermochim. Acta*, 1973, **6**, 275 (*ir, thermal anal*)
Htoon, S. *et al, J. Cryst. Mol. Struct.*, 1976, **6**, 55 (*struct*)

$C_6H_{16}CdI_2N_2$ IC-005258

Diiodo(*N,N,N',N'*-tetramethylethylenediamine)cadmium

Diiodo(N,N,N',N'-tetramethyl-1,2-ethanediamine-N,N')cadmium. (Tetramethylethylenediamine)cadmium diiodide
[28213-09-4]



M 482.4
Prob. has a distorted tetrahedral struct. Monomeric in soln. Air-stable colourless needles (MeOH). Mp 210-211°.
Abraham, M.H. *et al, Can. J. Chem.*, 1970, **48**, 181 (*ir, raman*)
Bell, N.A. *et al, Thermochim. Acta*, 1973, **6**, 275 (*synth, thermal stability*)
Armstrong, R.S. *et al, J. Mol. Struct.*, 1975, **29**, 117 (*solv, conform*)
Htoon, S. *et al, J. Cryst. Mol. Struct.*, 1976, **6**, 55 (*cryst struct*)

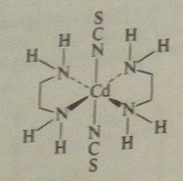
IC-005259

$C_6H_{18}CdN_6S_2$

Bis(ethylenediamine)diisothiocyanatocadmium

Bis(1,2-ethanediamine-N,N′)bis(thiocyanato-N)cadmium, 9CI. Cadmium(II) *isothiocyanate bis(ethylenediamine)*

[59433-36-2]



M 348.7

trans-Octahedral. Cryst. (EtOH). Sol. DMF.

Shvelashvili, A.E. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1974, **15**, 315 (*cryst struct*)

Diaz, A. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 2469 (*synth, ir, pmr*)

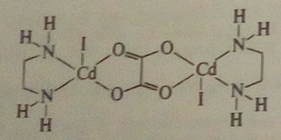
IC-005260

$C_6H_{16}Cd_2I_2N_4O_4$

Bis(ethylenediamine)diiodooxalatodicadmium

Bis(1,2-ethanediamine-N,N′)[μ-[ethanedioato(2−)-O,O″:O′,O‴]]diiododicadmium

[52654-19-0]



M 686.8

Tentative struct. shown. Cryst. (H_2O).

Shvelashvili, A.E. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1974, **19**, 553 (*synth, ir*)

IC-005261

$C_6H_{16}Cl_2HgN_2$

Dichloro(*N,N,N′,N′*-tetramethylethylenediamine)mercury

Dichloro(N,N,N′,N′-*tetramethyl-1,2-ethanediamine*-N,N′)*mercury*

[25725-91-1]

As Dibromo(*N,N,N′,N′*-tetramethylethylenediamine) mercury, IC-005255 with

X = Cl

M 387.7

Needles (MeOH). Sol. Me_2CO. Mp 162°.

[49662-43-3]

Coates, G.E. *et al*, *J. Chem. Soc.*, 1964, 160 (*synth, ir*)
Jain, S.C. *et al*, *Inorg. Chim. Acta*, 1969, **3**, 552 (*ir*)
Abraham, M.H. *et al*, *Can. J. Chem.*, 1970, **48**, 181 (*synth, ir, raman*)
Bryukhova, E.V. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci.* (*Engl. Transl.*), 1973, **22**, 1846 (*nqr*)
Caulton, K.G., *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 533 (*synth, ms, pmr*)
Bell, N.A. *et al*, *Thermochim. Acta*, 1973, **6**, 275 (*thermal anal*)
Htoon, S. *et al*, *J. Cryst. Mol. Struct.*, 1976, **6**, 55 (*cryst struct*)

IC-005262

$C_6H_{16}Cl_2N_2Zn$

Dichloro(*N,N,N′,N′*-tetramethylethylenediamine)zinc

(*Tetramethylethylenediamine*)*zinc dichloride*

[28308-00-1]

As Dibromo(*N,N,N′,N′*-tetramethylethylenediamine)zinc, IC-005256 with

X = Cl

M 252.5

Distorted tetrahedral geometry about Zn. Needles (EtOH). Mp 177°.

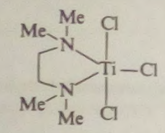
Coates, G.E. *et al*, *J. Chem. Soc.*, 1964, 166 (*synth, ir*)
Abrahams, M.H. *et al*, *Can. J. Chem.*, 1970, **48**, 181 (*synth, raman, ir*)
Caulton, K.G., *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 533 (*synth, ms, pmr*)
Armstrong, R.S. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1973, 1272, 1362 (*pmr*)
Htoon, S. *et al*, *J. Cryst. Mol. Struct.*, 1973, **3**, 95; 1976, **6**, 55 (*cryst struct*)
Bell, N.A. *et al*, *Thermochim. Acta*, 1973, **6**, 275 (*thermal anal*)

IC-005263

$C_6H_{16}Cl_3N_2Ti$

Trichloro(*N,N,N′,N′*-tetramethylethylenediamine) titanium(*III*)

[101050-01-5]



M 270.4

Synth. by heating the THF adduct to 60° in vacuum. Grey solid.

THF complex: [101050-00-4]. *Trichloro*(*tetrahydrofuran*)(N,N,N′,N′-*tetramethyl-1,2-ethanediamine*-N,N′)*titanium*(III), *11CI*

$C_{10}H_{24}Cl_3N_2OTi$ M 342.5

Synth. by reducing $TiCl_4$(tmed) with $LiBH_4$ in THF. Blue solid. Config. not reported.

Gordon, D. *et al*, *Inorg. Chim. Acta*, 1986, **111**, 77 (*synth, ir*)

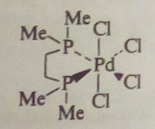
IC-005264

$C_6H_{16}Cl_4P_2Pd$

Tetrachloro[1,2-ethanediylbis[dimethylphosphine]-*P,P′*] palladium, 11CI

[*1,2-Bis*(*dimethylphosphino*)*ethane*]*tetrachloropalladium*(IV)

[85744-74-7]



M 398.3

Prepd. by chlorination of the dichloro compd. Orange cryst.

Gray, L.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 133 (*synth, ir*)

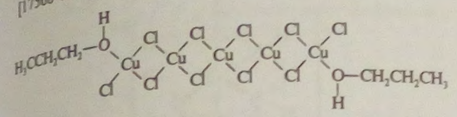
IC-005265

$C_6H_{18}Cl_{10}Cu_5O_2$

Decachlorobis(1-propanol)pentacopper(*II*)

Octa-μ-chlorodichlorobis(propyl alcohol)pentacopper, 8CI

[17568-08-0]



M 792.4

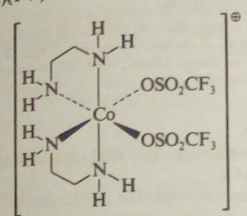
V. hygroscopic flat red plate-like cryst.

Willett, R.D. *et al*, *J. Chem. Phys.*, 1964, **40**, 838 (*synth, cryst struct*)
Willett, R.D., *J. Inorg. Nucl. Chem.*, 1967, **29**, 2482 (*uv*)

IC-005266

$C_6H_{16}CoF_6N_4O_6S_2^{\oplus}$

Bis(ethylenediamine-*N,N′*)bis(trifluoromethanesulfonato-*O*)cobalt(*III*)(1+)



M 477.2 (ion)

cis-form

Trifluoromethanesulfonate: [75522-52-0].
$C_9H_{16}CoF_9N_4O_9S_3$ M 626.3
Purple solid. Sol. H_2O.

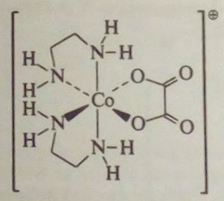
Dixon, N.E. *et al*, *Inorg. Chem.*, 1981, **20**, 470.
Inorg. Synth., 1983, **22**, 105 (*synth, uv*)

IC-005267

$C_6H_{16}CoN_4O_4^{\oplus}$

Bis(ethylenediamine)oxalatocobalt(*III*)(1+), 8CI

Bis(1,2-ethanediamine-N,N′)(*ethanedioato*-O,O′)*cobalt*(III) (*1+*)



M 267.1 (ion)

Chloride: [17439-00-8].
Sol. H_2O.

Andrade, C. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1328 (*synth*)
Andrade, C. *et al*, *Inorg. Chem.*, 1970, **9**, 711 (*synth, kinetics*)

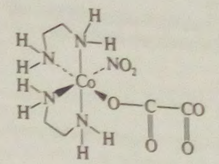
$C_6H_{16}CoN_5O_6$

IC-005268

Bis(ethylenediamine)(nitrito)oxalatocobalt(*III*)

Bis(1,2-ethanediamine-N,N′)(*ethanedioato*(2−)-O)(*nitrito*-N) *cobalt*(III), *11CI*

[85709-97-3]



cis-form

M 313.1

Octahedral with rare monodentate oxalate. Isomers distinguished by nmr.

cis-form

Dark orange solid. Spar. sol. H_2O.

trans-form [85760-73-2]

Orange solid. Sol. H_2O.

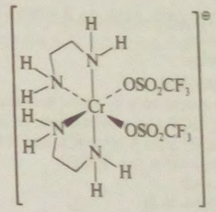
Cooper, J.N. *et al*, *Inorg. Chem.*, 1983, **22**, 1956 (*synth, ir, uv, pmr, cmr*)

IC-005269

$C_6H_{16}CrF_6N_4O_6S_2^{\oplus}$

Bis(ethylenediamine)bis(trifluoromethanesulfonato) chromium(*III*)(1+)

Bis(1,2-ethanediamine-N,N′)*bis(trifluoromethanesulfonato*-O) *chromium*(III)(*1+*), *11CI*



M 470.3 (ion)

cis-Octahedral.

Trifluoromethanesulfonate: [90065-91-1].
Pink powder. Stable in dry air, dec. slowly in light. Sensitive to prolonged heating.

Dixon, N.E. *et al*, *Inorg. Chem.*, 1984, **23**, 2940 (*synth, ir, uv-vis, kinetics*)
Inorg. Synth., 1986, **24**, 250 (*synth*)

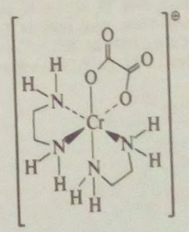
IC-005270

$C_6H_{16}CrN_4O_4^{\oplus}$

Bis(ethylenediamine)oxalatochromium(*III*)(1+), 8CI

Bis(1,2-ethanediamine-N,N′)[*ethanedioato*(2−)-O,O′] *chromium*(III)(*1+*), *11CI, 10CI, 9CI*

[21748-30-1]



Δ-*form*

M 260.2 (ion)

Octahedral complex: (+)-form assigned as Λ config. (−)-form assigned to Δ config.

Chloride: [29046-77-3].

Perchlorate: [42423-95-0].
Orange cryst. (H_2O).
▷ Potentially explosive.

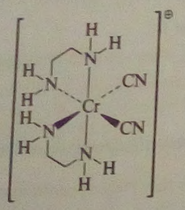
(Ethylenediamine)bis(oxalato)chromate(III) *salt:* see *(Ethylenediamine)bis(oxalato)chromate*(III)(1−), IC-005016

[29753-90-0, 36538-25-7]

Lethbridge, J.W. *et al, J. Chem. Soc. A*, 1970, 1862 (*cryst struct, double salt*)
House, D.A. *et al, Inorg. Chim. Acta*, 1982, **60**, 145 (*resoln, perchlorate*)

$C_6H_{16}CrN_6^{\oplus}$ IC-005271

Biscyanobis(ethylenediamine)chromium(*III*)(1+)
Bis(cyano-C)bis(1,2-ethanediamine-N,N′)chromium(III) *(1+), 11Cl 10Cl, 9Cl*



cis-form

M 224.2 (ion)
Isomeric mixture synth. from aq. $[Cr(en)_3]Cl_3$ and NaCN.

cis-form [53302-06-0]
Aquates readily.

Chloride: [58602-38-3].
Synth. from perchlorate by anion exchange; or from $CrCl_3.6H_2O$, KCN and ethylenediamine in hot MeOH with Zn dust; or from $[Cr(en)_3]Cl_3$ and KCN in warm DMSO. Yellow cryst. (aq. EtOH).

Iodide: [58602-37-2].

Perchlorate: [55659-58-0].
Synth. from chloride and aq. $NaClO_4$. Yellow cryst. (MeOH aq.). More sol. in H_2O than *trans*-salt.

trans-form [72074-79-4]
trans-Salts not easily obtained.

Chloride: Synth. from perchlorate by anion exchange.

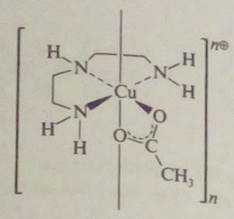
Perchlorate: [72074-80-7].
Yellow cryst. (MeOH aq.). Less sol. than corresp. salt of *cis*-isomer.

[55659-57-9, 55659-59-1, 56848-41-0, 58602-40-7, 58641-32-0, 97485-63-7]

Kaizaki, S. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 902 (*synth, resoln, ir, uv, cd*)
Maki, N., *J. Inorg. Nucl. Chem.*, 1975, **37**, 1207 (*electrochem*)
Sattelberger, A.P. *et al, Inorg. Chem.*, 1976, **15**, 1412 (*synth, uv, ir, resolution*)
Kirk, A.D. *et al, Inorg. Chem.*, 1980, **19**, 445 (*synth, photol*)
Heatherington, A. *et al, Inorg. Chim. Acta*, 1980, **44**, L279.
Kirk, A.D. *et al, J. Phys. Chem.*, 1980, **84**, 887.
Sakabe, Y. *et al, Inorg. Chem.*, 1985, **24**, 2119 (*synth, resoln*)

$C_6H_{16}CuN_3O_2^{\oplus}$ IC-005272

Acetato(diethylenetriamine)copper(*II*)(1+)
(Acetato-O)[N-(2-aminoethyl)-1,2-ethanediamine-N,N′,N″]copper(1+), 11Cl



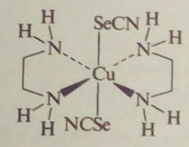
M 225.7 (ion)
Chain struct. with Cu(*II*) ions linked by bridging acetate groups, Cu-O 240, 265 pm.

Perchlorate: [21279-30-1].
Deep blue cryst. (hot MeOH). Insol. EtOH, Et_2O.
▷ Potentially explosive.

Curtis, N.F., *J. Chem. Soc. A*, 1968, 1579 (*synth, ir, uv, magnetism*)
Manhas, B.S. *et al, J. Indian Chem. Soc.*, 1982, **59**, 315 (*ir*)
Towle, D.K. *et al, Inorg. Chem.*, 1988, **27**, 394 (*cryst struct, synth, esr*)

$C_6H_{16}CuN_6Se_2$ IC-005273

Bis(1,2-ethanediamine-*N,N′*)bis(selenocyanato-*Se*)copper(*II*), 11Cl
Bis(ethylenediamine)copper(II) *selenocyanate*

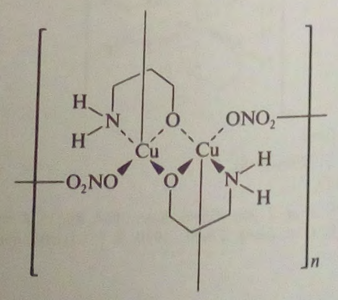


M 393.6
trans-Octahedral. Flat blue-purple cryst. Sol. polar solvs.

Vrabel, V. *et al, Collect. Czech. Chem. Commun.*, 1983, **48**, 2893 (*synth, cryst struct*)

$C_6H_{16}Cu_2N_4O_8$ IC-005274

Bis[μ-(3-amino-1-propanolato-*N,O:O*)]bis(nitrato-*O*)dicopper(*II*), 12Cl
[130034-14-9]



M 399.3
Each Cu has distorted square pyramidal coordination with a nitrate from the adjacent dimer apical. Dark blue cryst. Insol. EtOH, Me_2CO.

Lindgren, T. *et al, Inorg. Chim. Acta*, 1990, **171**, 95 (*synth, cryst struct, magnetism*)

$C_6H_{16}HgI_2N_2$ IC-005275

Diiodo(*N,N,N′,N′*-tetramethylethylenediamine)mercury
Diiodo(N,N,N′,N′-tetramethyl-1,2-ethanediamine-N,N′)mercury

[26758-71-4]
As Dibromo(*N,N,N′,N′*-tetramethylethylenediamine) mercury, IC-005255 with

X = I

M 570.6
Needles (MeOH). Mp 162°.

[49662-45-5]

Abraham, M.H. *et al, Can. J. Chem.*, 1970, **48**, 181 (*synth, ir, raman*)
Bryukhova, E.V. *et al, Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1973, **22**, 1846 (*nqr*)
Bell, N.A. *et al, Thermochim. Acta*, 1973, **6**, 275 (*thermal anal*)
Htoon, S. *et al, J. Cryst. Mol. Struct.*, 1976, **6**, 55 (*cryst struct*)

$C_6H_{16}I_2N_2Zn$ IC-005276

Diiodo(*N,N,N′,N′*-tetramethylethylenediamine)zinc
(Tetramethylethylenediamine)zinc diiodide

[14726-56-8]
As Dibromo(*N,N,N′,N′*-tetramethylethylenediamine)zinc, IC-005256 with

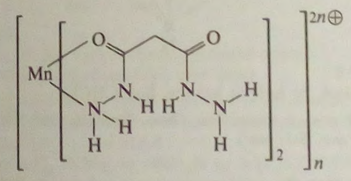
X = I

M 435.4
Needles (MeOH or THF). Mp 201-202°.

Abraham, M.H. *et al, J. Organomet. Chem.*, 1967, **7**, 35 (*synth*)
Bell, N.A. *et al, Thermochim. Acta*, 1973, **6**, 275 (*synth, thermal anal*)
Abraham, M.H. *et al, Can. J. Chem.*, 1974, **48**, 181 (*synth, ir, raman*)
Htoon, S. *et al, J. Cryst. Mol. Struct.*, 1974, **4**, 357; 1976, **6**, 55 (*cryst struct*)

$C_6H_{16}MnN_8O_4^{2\oplus}$ IC-005277

Bis(propanedioic acid dihydrazide)manganese(2+), 11Cl
Bis(μ-dihydrazidomalonate-N,N′,O,O′)manganese(2+)



M 319.1 (ion)
Both α- and β-forms comprise polymeric chain cations of 8-coordinate Mn. In α-form, coordn.geometry is intermed. between dodecahedral and square antiprismatic; in β-form polyhedron is square antiprismatic. Synth. from saturated aq. solns. of the manganese salts and ligand.

Dichloride: [98478-84-3].
Light yellow cryst. $+2H_2O$. Mp 128°. $\mu_{eff} = 5.64\mu_B$ (297K).

Sulfate: [96411-16-4].
Light yellow cryst. $+ 4H_2O$. Mp 191°. $\mu_{eff} = 6.13\mu_B$ (297K).

Dutta, A. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 2951; 1969, **31**, 2545 (*synth, ir, magnetism, uv, props*)
Vardosanidze, T.O. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1985, **30**, 203, 992 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 200 (*rev, bibl*)

$C_6H_{16}MnN_{10}O_4S_2$ IC-005278

Bis(thiocyanato-*N*)tetrakis(urea-*O*)manganese(*II*), 10Cl
Bis(thiocyanato-N)tetra(urea)manganese(II)
[42427-90-7]

$Mn(NCS)_2[O{=}C(NH_2)_2]_4$

M 411.3
trans-Octahedral complex. Synth. from $Mn(NCS)_2$, urea and $HC(OEt)_3$ in refluxing anhydrous EtOH under N_2. Colourless cryst. ($EtOH/Et_2O$), gradually oxidises and blackens in air. Sol. H_2O, EtOH, MeOH, Et_2O, Me_2CO, and DMF. Sl. sol. CCl_4, C_6H_6. Mp 141°. $\mu_{eff} = 5.88\mu_B$.

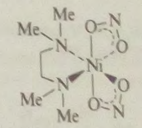
Tetrakis-urea adduct: [67269-92-5].
$C_{10}H_{32}MnN_{18}O_8S_2$ M 651.5
Synth. from $Mn(NCS)_2$ and urea (mole ratio 1:8) in dry refluxing EtOH under N_2 with addition of $HC(OEt)_3$. Colourless solid. Mp 120°. $\mu_{eff} = 5.87\mu_B$.

Tsintsadze, G.V. *et al, CA*, 1973, **79**, 73060 (*props*)
Tsintsadze, G.V. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1974, **5**, 282 (*cryst struct*)
Barbier, J.P. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 2283 (*synth, uv, esr, ir, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 145 (*rev, bibl*)

$C_6H_{16}N_4NiO_4$ IC-005279

Dinitro(*N,N,N′,N′*-tetramethylethylenediamine)nickel(*II*)
Bis(nitrito-O,O′)(N,N,N′,N′-tetramethyl-1,2-ethanediamine-N,N′)nickel, 9Cl

[14267-06-2]



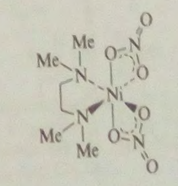
M 266.9
Octahedral structure with chelating $NO_2^{\ominus}$. Distorted from regularity by steric restrictions of $NO_2^{\ominus}$. Green cryst. Paramagnetic.

Goodgame, D.M.L. *et al, Inorg. Chem.*, 1965, **4**, 721 (*synth, ir, uv, magnetism*)
Drew, M.G.B. *et al, J. Chem. Soc., Chem. Commun.*, 1965, 476 (*struct*)
Finney, A.J. *et al, Aust. J. Chem.*, 1981, **34**, 2159.

$C_6H_{16}N_4NiO_6$ IC-005280

(Dinitrato-*O,O′*)(*N,N,N′,N′*-tetramethylethylenediamine)nickel(*II*), 8Cl
Dinitrato(N,N,N′,N′-*tetramethyl-1,2-ethanediamine*)*nickel, 9Cl*

[14878-50-3]

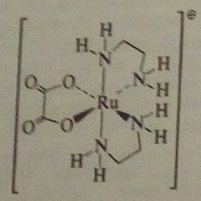


M 298.9
Octahedral struct. with bidentate $NO_3^{\ominus}$. Similar compds. known for other diamines. Synth. from $Ni(NO_3)_2$ + $Me_2NCH_2CH_2NMe_2$. Turquoise solid. Sol. polar org. solvs. Mp 176-178°. Paramagnetic.

Sacconi, L. *et al*, *Inorg. Chem.*, 1967, **6**, 262 (*synth, ir, uv, magnetism*)
Turpeinen, U., *Suom. Kem. B*, 1973, **46**, 308 (*struct*)

$C_6H_{16}N_4O_4Ru^{\oplus}$ IC-005281

Bis(ethylenediamine)oxalatoruthenium(*III*)(1+)
(Oxalato)bis(1,2-diaminoethane)ruthenium(III)(*1+*). *Bis(1,2-ethanediamine-N,N′)[ethanedioato(2−)-O,O′]ruthenium*(III) (*1+*), *9CI*
[46360-66-1]

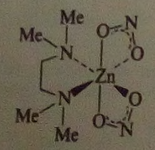


M 309.2 (ion)
Sol. H_2O.
Iodide: Orange salt + $\frac{1}{2}H_2O$.
Tetraphenylborate: Yellow salt + $2H_2O$.
Ethylenediaminebis(oxalato)ruthenate(1−) salt:
$C_{12}H_{24}N_6O_{12}Ru_2$ M 646.4
Yellow cryst. μ_{eff} = 2.16μ_B (per Ru atom).

Broomhead, J.A. *et al*, *J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, magnetism*)

$C_6H_{16}N_4O_4Zn$ IC-005282

Bis(nitrito-*O,O′*)(*N,N,N′,N′*-tetramethyl-1,2-ethanediamine-*N,N′*)zinc, 10CI
[81174-46-1]

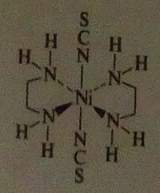


M 273.6
Octahedral Zn. Cryst. (MeOH).

Finney, A.J. *et al*, *Aust. J. Chem.*, 1981, **34**, 2159 (*ir, cryst struct*)
Goodgame, D.M.L. *et al*, *J. Chem. Soc. A*, 1970, 1933 (*synth, ir*)

$C_6H_{16}N_6NiS_2$ IC-005283

Bis(ethylenediamine)bis(thiocyanato-*N*)nickel(*II*)
Diisothiocyanatobis(ethylenediamine)nickel(II). *Bis(1,2-ethanediamine)bis(thiocyanato-N)nickel, 9CI*
[15555-47-2]

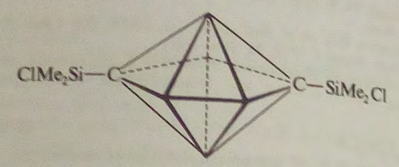


M 295.0
Octahedral, only found as *trans*-config.
trans-NCS-form [15602-85-4]
Blue-violet monoclinic plates (H_2O).
[20658-28-0]

Brown, B.N. *et al*, *Acta Crystallogr.*, 1963, **16**, 753 (*synth, struct*)
Lever, A.B.P. *et al*, *Can. J. Chem.*, 1973, **51**, 1567 (*ir*)
Bertini, I. *et al*, *Inorg. Chem.*, 1976, **15**, 203 (*uv*)

$C_6H_{17}B_3Cl_2Si_2$ IC-005284

2,4-Bis(chlorodimethylsilyl)-2,4-dicarbaheptaborane(7), 10CI
[28699-83-4]

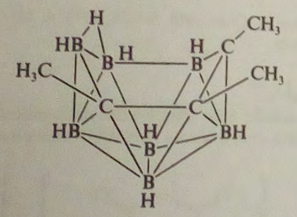


M 270.3
closo-. Monomer used for polymer formation. Colourless liq. Mp −14.9°. Bp 234.4°.

Kesting, R. *et al*, *J. Appl. Polym. Sci.*, 1970, **14**, 2525.
Zhigach, A. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1978, **48**, 536 (*ir, ms*)
Golosova, R. *et al*, *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1979, **53**, 435.

$C_6H_{17}B_7$ IC-005285

5,6,10-Trimethyl-5,6,10-tricarbadecaborane(11)
[114901-05-2]

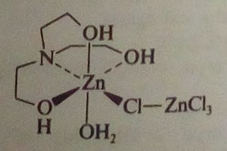


M 164.8
nido-. Isol. by hplc in hexane. Sol. $CHCl_3$.

Stibr, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 1106 (*synth, pmr, cmr, B-11 nmr*)

$C_6H_{17}Cl_4NO_4Zn_2$ IC-005286

Aqua(triethanolamine)tetrachlorodizinc
*Aqua-μ-chlorotrichloro[2,2′,2″-nitrilotris[ethanol]-*N,O,O′,O″] *dizinc, 9CI*
[29977-30-8]

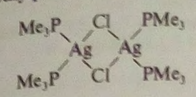


M 439.7
Distorted octahedral and tetrahedral Zn environments. Hygroscopic cryst. (aq. EtOH).

Follner, H., *Z. Anorg. Allg. Chem.*, 1972, **387**, 43 (*cryst struct*)

$C_6H_{18}AgClP_2$ IC-005287

Chlorobis(trimethylphosphine)silver



M 295.4
Dimeric.
Dimer: [40696-74-0]. *Di-μ-chlorotetrakis(trimethylphosphine) disilver, 9CI*
$C_{12}H_{36}Ag_2Cl_2P_4$ M 590.9
Cryst. (C_6H_6/pet. ether). Sol. C_6H_6. Mp 75°.

Schmidbaur, H. *et al*, *Chem. Ber.*, 1972, **105**, 3382 (*synth*)

$C_6H_{18}AgN_{10}^{3\oplus}$ IC-005288

Bis(1-methylbiguanidine)silver(*III*)(3+)
*Bis(methylimidodicarbonimidic diamide-*N″,N‴*)silver(3+)*
As Bis(biguanidine)silver(*III*)(3+), IC-004290 with

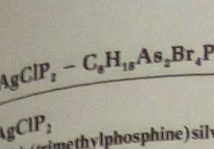
R = Me

M 338.1 (ion)
Square planar at Ag. Varying degrees of salt solubility in H_2O. Insol. most org. solvs.
Trihydroxide: [24899-86-3].
Dark brown powder. Spar. sol. H_2O; insol. org. solvs.
Trinitrate: Yellow cryst. Sol. H_2O; insol. org. solvs.

Sen, D., *J. Chem. Soc.*, 1969, 1304 (*synth, magnetism*)
Swartz, W.E. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1974, **4**, 351 (*pe*)

$C_6H_{18}AlN_3$ IC-005289

Tris(dimethylamido)aluminium
Tris(dimethylamino)alane



Dimer

M 159.2
Dimeric. V. sol. hydrocarbons. Related compd. $Al(NMe_2)_2NH$(adamantyl) also descr.
Dimer: [32093-39-3]. *Bis[μ-(N-methylmethanaminato)] tetrakis(N-methylmethanaminato)dialuminium, 11CI*
$C_{12}H_{36}Al_2N_6$ M 318.4
From $AlH_3.2NMe_3$ + NMe_2H or $Al[CH_2CH(CH_3)_2]_3$ + NMe_2H. Colourless moisture-sensitive cryst. (by subl.). Sol. Et_2O, C_6H_6. Mp 87-88°. Subl.$_{0.001}$ 90°.

Wiberg, E. *et al*, *Z. Naturforsch., B*, 1955, **10**, 234 (*synth*)
Longi, P. *et al*, *Gazz. Chim. Ital.*, 1960, **90**, 180 (*synth*)
Ruff, J.K. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2835 (*synth, reactions*)
Kovar, R.A. *et al*, *Inorg. Chem.*, 1973, **10**, 893 (*pmr*)
Keller, P.C., *J. Am. Chem. Soc.*, 1974, **96**, 3073 (*reactions*)
Ouzounis, K. *et al*, *Z. Anorg. Allg. Chem.*, 1983, **504**, 67 (*cryst struct, pmr, ir, raman*)
Waggoner, K.M. *et al*, *Polyhedron*, 1990, **9**, 257 (*synth, cryst struct*)

$C_6H_{18}AsN_3$ IC-005290

Tris(dimethylamino)arsine, 8CI
Hexamethylarsenous triamide, 9CI. Tris(dimethylamido) arsenic
[6596-96-9]

$As(NMe_2)_3$

M 207.1
Reacts with aldehydes or ketones to give enamines and/or *gem*-diamines. Complexes with Group VIB carbonyls. Reacts with alcohols to give arsenite esters. Liq. d_4^{20} 1.12. Mp −53°. Bp 170° (extrap.), Bp_{10} 54°, $Bp_{3.5}$ 42-43°. n_D^{20} 1.4848.

Mödritzer, K., *Chem. Ber.*, 1959, **92**, 2637 (*synth, ir*)
Weingarter, H. *et al*, *J. Org. Chem.*, 1966, **31**, 4041 (*props, use*)
Von Hirsch, H., *Chem. Ber.*, 1967, **100**, 1289 (*synth, props, use*)
Inorg. Synth., 1967, **10**, 131 (*synth, pmr*)
King, R.B. *et al*, *Inorg. Chem.*, 1971, **10**, 1188 (*derivs*)
Mason, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2337 (*N-15 nmr*)
Davidson, G. *et al*, *Spectrochim. Acta, Part A*, 1979, **35**, 141 (*ir, raman*)
Bergesen, K. *et al*, *Acta Chem. Scand., Ser. A*, 1981, **35**, 147 (*cmr*)

$C_6H_{18}As_2Br_2FeO_2$ IC-005291

Dibromobis(trimethylarsine oxide)iron(*II*)
Iron(II) *bromide bis(trimethylarsine oxide)*
[25668-88-6]

$[FeBr_2(O{=}AsMe_3)_2]_n$

M 487.7
Polymeric with octahedral Fe(*II*) and bridging ligands. Synth. from $FeBr_2$ + Me_3AsO in hot EtOH or Me_2CO. Buff coloured solid; oxidises in air.

Brodie, A.N. *et al*, *J. Chem. Soc. A*, 1969, 1931 (*synth, ir, uv*)

$C_6H_{18}As_2Br_2FeS_2$ IC-005292

Dibromobis(trimethylarsine sulfide)iron(*II*)
Iron(II) *bromide bis(trimethylarsine sulfide)*
[26233-62-5]

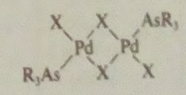
$FeBr_2(S{=}AsMe_3)_2$ (C_{2v})

M 519.8
Synth. from $FeBr_2$ + Me_3AsS in hot EtOH or Me_2CO. Buff solid; rel. stable in air; oxidises in soln. Sol. $MeNO_2$, CH_2Cl_2.

Brodie, A.N. *et al*, *J. Chem. Soc. A*, 1969, 1931 (*synth, ir, uv*)

$C_6H_{18}As_2Br_4Pd_2$ IC-005293

Di-μ-bromodibromobis(trimethylarsine)dipalladium(*II*), 8CI
Tetrabromobis(trimethylarsine)dipalladium(II)
[21259-05-2]



R = Me, X = Br

M 772.5
Probably has *trans*-configuration with 2 bridging Br and square planar Pd, as shown. Synth. from Tetrabromopalladate(*II*)(2−), IC-002064 + $PdBr_2(AsMe_3)_2$. Sol. CH_2Cl_2.

Monomer. Dibromo(trimethylarsine)palladium. Palladium(II) bromide trimethylarsine
$C_3H_9AsBr_2Pd$ M 386.2
Unknown.

Chatt, J. et al. J. Chem. Soc., 1957, 2351 (synth method)
Duddell, D.A. et al. J. Chem. Soc. A, 1969, 2134; 1970, 545 (pmr, ir, raman)

IC-005294

$C_6H_{18}As_2Cl_2FeO_2$
Dichlorobis(trimethylarsine oxide)iron(II)
Iron(II) chloride bis(trimethylarsine oxide)
[25668-87-5]

$[FeCl_2(O{=}AsMe_3)_2]_n$

M 398.8
Polymeric with octahedral Fe(II) and bridging chloride ligands. Synth. from $FeCl_2$ + Me_3AsO in hot Me_2CO or EtOH. Buff solid; oxidises in air.

Brodie, A.N., J. Chem. Soc. A, 1969, 1931 (synth, ir, str)

IC-005295

$C_6H_{18}As_2Cl_2FeS_2$
Dichlorobis(trimethylarsine sulfide)iron(II)
Iron(II) chloride bis(trimethylarsine sulfide)
[26233-61-4]

$FeCl_2(S{=}AsMe_3)_2$ (C_{2h})

M 430.9
Synth. from $FeCl_2$ + Me_3AsS in hot EtOH or Me_2CO. Buff solid; rel. stable in air; oxidises in $MeNO_2$, CH_2Cl_2. Sol. $MeNO_2$, CH_2Cl_2 (dec.).

Brodie, A.N. et al, J. Chem. Soc. A, 1969, 1931 (synth)

IC-005296

$C_6H_{18}As_2Cl_2Pd$
Dichlorobis(trimethylarsine)palladium(II)
[21292-65-9]

$PdCl_2(AsMe_3)_2$

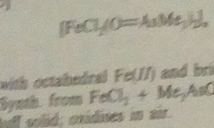
M 417.3
Exists as *cis*-square planar isomer in solid state. Yellow solid (EtOH/Me_2CO). Mp 234-235° (236°). Ir ν_{Pd-Cl} 317, 299 cm^{-1}.

[23627-44-3]

Coates, G.E. et al, J. Chem. Soc., 1963, 421 (ir)
Goodfellow, R.J. et al, J. Chem. Soc. A, 1968, 1604 (ir, synth)
Mann, F.G. et al, J. Chem. Soc., 1935, 1549 (synth)
Park, P.J.D. et al, Spectrochim. Acta, Part A, 1969, 25, 227 (ir, raman)

IC-005297

$C_6H_{18}As_2Cl_3PtSn_3^{\ominus}$
Tris(trichlorostannyl)bis(trimethylarsine)platinate(1−)
Tris(trichlorotin)bis(trimethylarsine)platinate(1−)

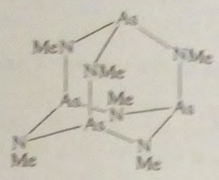


M 1110.3 (ion)
Bis(triphenylphosphine)iminium salt: Cryst. (Me_2CO).

Albinati, A. et al, Angew. Chem., Int. Ed. Engl., 1982, 21, 284 (synth, nmr, struct)

IC-005298

$C_6H_{18}As_4N_6$
2,4,6,8,9,10-Hexamethyl-2,4,6,8,9,10-hexaaza-1,3,5,7-tetraarsaadamantane
2,4,6,8,9,10-Hexamethyl-2,4,6,8,9,10-hexaaza-1,3,5,7-tetraarsatricyclo[3.3.1.1^{3,7}]decane, 9CI
[2030-90-2]



M 473.9
Adamantane-like struct. Mean As—N 187 pm. Synth. from $AsCl_3$ + $MeNH_2$. Mod. sol. H_2O, $CHCl_3$, C_6H_6, sl. sol. toluene, Me_2CO, EtOH. Mp 122-132° (range). Cleaved by acid eg. CF_3SO_3H, with loss of $MeNH_2$.

Holmes, R.R. et al, Inorg. Chem., 1963, 2, 377 (synth, pmr)
Vetter, H.-J. et al, Z. Anorg. Allg. Chem., 1964, 329, 144 (synth)
Weiss, J. et al, Z. Anorg. Allg. Chem., 1967, 350, 9 (cryst struct)
Wolff, A. et al, Org. Mass Spectrom., 1974, 9, 594 (ms)
Postel, M. et al, Inorg. Chim. Acta, 1976, 17, L23 (pmr, props)

IC-005299

$C_6H_{18}AuO_4P_2^{\oplus}$
Bis(trimethyl phosphite)gold(1+)
[82598-60-5]

$Au[P(OMe)_3]_2^{\oplus}$

M 445.1 (ion)
Perchlorate:
$C_6H_{18}AuClO_{10}P_2$ M 544.5
Cryst. ($CHCl_3$/Et_2O). Sol. $CHCl_3$.

Chastain, S.K. et al, Inorg. Chem., 1982, 21, 3717 (synth, mol)

IC-005300

$C_6H_{18}BN$
Trihydro(triethylamine)boron
Borane triethylamine. (N,N-Diethylethanamine) trihydroboron, 10CI. Triethylamine borane
[1722-26-5]

$Et_3N{-}BH_3$

M 115.0
Liq. with camphor-like odour. d_{20} 0.785. Mp −2°. Bp_{12} 100-101°.

Köster, R., Angew. Chem., 1957, 69, 94 (synth)
Zigach, A.F., Zh. Obshch. Khim., 1957, 27, 1655 (synth)
Heitsch, C.W., Inorg. Chem., 1965, 4, 1019 (nmr)
Faulks, J.N.G. et al, J. Inorg. Nucl. Chem., 1967, 29, 329 (ir, nmr)
Purser, J.M. et al, Inorg. Chem., 1968, 7, 2156 (nmr)
Sheikh, S.U., J. Math. Sci., 1974, 1, 131 (ms)

IC-005301

$C_6H_{18}BNO$
[(2-Ethoxyethyl)dimethylamine]trihydroboron
Borane 2-ethoxy-N,N-dimethylethylamine. (2-Ethoxy-N,N-dimethylethanamine-N)trihydroboron, 10CI. 2-Ethoxy-N,N-dimethylethanamine compd. with borane (1:1)
[67036-04-8]

$EtOCH_2CH_2NMe_2{-}BH_3$

M 131.0

U.S. Pat., 4 080 381, (1978); CA, 89, P23753z.
U.S. Pat., 4 142 902, (1979); CA, 91, P25752p.

IC-005302

$C_6H_{18}B_2N_2O_2$
1,2-Dimethoxy-1,2-bis(dimethylamino)diborane(4)
1,2-Dimethoxy-N,N,N′,N′-tetramethyl-1,2-diborane(4) diamine, 10CI, 9CI
[4285-34-3]

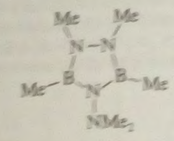
$Me_2NB(OMe){-}B(OMe)NMe_2$

M 170.8
No phys. props. reported but probably liq., sensitive to moist air.

Nöth, H. et al, Chem. Ber., 1973, 106, 1145 (nmr)
Biffar, W. et al, Chem. Ber., 1980, 113, 333 (nmr)

IC-005303

$C_6H_{18}B_3N_3$
4-(Dimethylamino)-1,2,3,5-tetramethyl-1,2,4,3,5-triazadiborolidine, 8CI
N,N,1,2,3,5-Hexamethyl-1,2,4,3,5-triazadiborolidin-4-amine, 10CI, 9CI. 4-Dimethylamino-1,2,3,5-tetramethyl-1,2,4,3,5-triazadiborolane. 4-Dimethylamino-1,2,3,5-tetramethyl-1,2,4-triaza-3,5-diboracyclopentane
[3732-42-0]



M 167.8
Liq., somewhat sensitive to moist air. Bp_{15} 74°, Bp_{12} 62°. ^{11}B nmr δ −31.0 ppm.

Nöth, H. et al, Angew. Chem., Int. Ed. Engl., 1971, 10, 126 (synth, props, B-11 nmr)
Nöth, H. et al, Z. Anorg. Allg. Chem., 1974, 406, 235.
Nöth, H. et al, Chem. Ber., 1979, 112, 2494 (pmr, props)

IC-005304

$C_6H_{18}B_3N_3$
Hexamethylborazine, 10CI, 9CI
Hexahydrohexamethyl-s-triazatriborine. Hexamethyltriborinetriamine. Hexamethylborazole
[877-07-6]

As Borazine, IC-001044 with

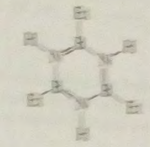
R = R′ = Me

M 164.6
Air-stable cryst. (MeCN). Sol. hexane, $CHCl_3$. Mp 98-99°. Bp 221°. High thermal stability; mod. hydrolytic stability in neutral soln.

Wiberg, E. et al, Z. Anorg. Allg. Chem., 1947, 255, 141 (synth)
Haworth, D.T. et al, J. Am. Chem. Soc., 1960, 82, 3860 (synth)
Butcher, I.M. et al, J. Chem. Soc., 1964, 4528 (synth, pmr)
Meicher, L.A. et al, Inorg. Chem., 1972, 11, 1247; 1973, 12, 601 (ir, ms)
Wrackmeyer, B. et al, Chem. Ber., 1976, 109, 3480 (nmr)
Nöth, H. et al, Chem. Ber., 1981, 114, 1150 (nmr)

IC-005305

$C_6H_{18}B_3N_3$
2,4,6-Triethylborazine, 10CI, 9CI, 8CI
B,B,B-Triethylborazole
[7445-22-3]



M 164.6
Liq. with unpleasant odour. Sol. most org. solvs. d_4^{20} 0.866. Fp −54° to −53°, −46.4°. Bp. 66-67°. Viscosity 1.48 centistokes at 20°. ΔH°_{vap} 40.5 kJ mol^{-1}. Trouton const. 22.1 e.u. Dec. > 100°, stable to water at r.t. Vp 3.35 mm at 26.6°.

Haworth, D.T. et al, J. Am. Chem. Soc., 1960, 82, 3860 (ir, synth)
Hawthorne, M.F. et al, J. Am. Chem. Soc., 1961, 83, 859 (ac, ir, nmr, synth)
Köster, R. et al, Justus Liebigs Ann. Chem., 1961, 648, 1 (ir, synth)
Powell, P. et al, J. Chem. Soc., 1964, 288 (synth, chromatog)
Nöth, H. et al, J. Organomet. Chem., 1968, 12, 23 (pmr)
Wrackmeyer, B. et al, Chem. Ber., 1976, 109, 3480 (nmr)
Nöth, H. et al, Chem. Ber., 1981, 114, 1150 (nmr)

IC-005306

$C_6H_{18}Br_2CrO_3S_3$
Dibromotris(dimethyl sulfoxide)chromium(II)
Chromium(II) bromide tris(dimethyl sulfoxide)

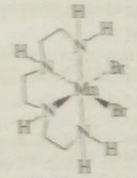
$CrBr_2(O{=}SMe_2)_3$

M 446.2
Struct. unknown. Pale blue cryst. (EtOH). μ_{eff} = 4.96μ_B (293K).

Holah, D.G. et al, Inorg. Chem., 1965, 4, 1722 (synth, ac, ir)

IC-005307

$C_6H_{18}Br_2MnN_4$
Dibromo(triethylenetetramine)manganese(II)



M 360.9
High spin manganese(II) complex, assumed to be octahedral. μ_{eff} = 5.87μ_B (295K). Synth. from 1:1 mole ratios of $MnBr_2.H_2O$ and trien in EtOH. Yellow cryst. Non-electrolyte in $MeNO_2$.

Chiswell, B., Inorg. Chim. Acta, 1975, 12, 195 (synth, magnetism, cond)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, D3, 58 (rev, bibl)

IC-005308

$C_6H_{18}Br_2NiP_2$
Dibromobis(trimethylphosphine)nickel(II)
[20663-83-6]

$NiBr_2(PMe_3)_2$

M 370.6
Square planar.

trans-form [38907-48-1]
Dark red microcryst.

[19615-75-9]

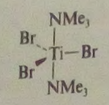
Meier, P.F. *et al, Inorg. Chem.*, 1979, **18**, 610 (*props, struct, bibl, spectra*)
Mari, A. *et al, Inorg. Chim. Acta*, 1981, **52**, 83 (*synth, cryst struct*)

IC-005309

$C_6H_{18}Br_3N_2Ti$

Tribromobis(trimethylamine)titanium(*III*)
Tribromobis(N,N-*dimethylmethanamine*)*titanium*(III), *9CI*.
Titanium(III) *bromide bis(trimethylamine)*

[14875-38-8]



M 405.8
Probably only *trans*-form exists. Synth. by reducing $TiBr_4$ with excess NMe_3 or by dissolving $TiBr_3$ in NMe_3.

trans-form [24150-56-9]
Tbp with *trans* amines, actual symmetry is C_{2v}. Green solid. Sol. C_6H_6. Paramagnetic, $\mu_{eff} = 1.67\ \mu_B$ (293K).

Fowles, G.W.A. *et al, J. Chem. Soc.*, 1963, 33 (*synth*)
Crouch, P.C. *et al, J. Chem. Soc. A*, 1968, 2172 (*uv-vis, ir*)
Wood, J.S. *et al, Inorg. Chem.*, 1969, **8**, 491 (*magnetism, uv-vis, cryst field calcs*)
Greene, P.T. *et al, J. Chem. Soc. A*, 1971, 3636 (*cryst struct, trans-form*)

IC-005310

$C_6H_{18}Br_3N_2V$

Tribromobis(trimethylamine)vanadium(*III*), 8CI
Tribromobis(*dimethylmethanamine*)*vanadium*(III), *9CI*.
Vanadium(III) *bromide bis(trimethylamine)*

[20538-62-9]

$$VBr_3(NMe_3)_2$$

M 408.8
Trigonal-bipyramidal. Synth. from VBr_3 + pure Me_3N. $VBr_3.Me_3N$ is also formed. Pink solid. Sol. Me_3N, C_6H_6.

trans-form [19631-73-3]
Identified by physical props. and by analogy with chloro complex. Pink solid. Sol. Me_3N, C_6H_6.

Duckworth, M.W. *et al, J. Chem. Soc. A*, 1967, 1592 (*synth, uv-vis, ir, dipole moment*)
Wood, J.S., *Inorg. Chem.*, 1968, **7**, 852 (*uv-vis*)
Crouch, P.C. *et al, J. Chem. Soc. A*, 1968, 2172 (*uv-vis, ir*)

IC-005311

$C_6H_{18}CeCl_4O_3S_3$

Tetrachlorotris(dimethyl sulfoxide)cerium(*IV*)
Tetrachlorotris[*sulfinylbis*[*methane*]-O]*cerium*(IV), *11CI*.
Cerium(IV) *chloride tris(dimethyl sulfoxide)*

[35163-49-6]

$$CeCl_4(O{=}SMe_2)_3$$

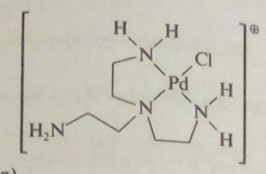
M 516.3
Possibly exists as $[Ce(Me_2SO)_6Cl_2]^{2\oplus}[CeCl_6]^{2\ominus}$ by analogy with similar compds. of U. V. hygroscopic orange or red solid. Sol. CH_2Cl_2, $MeNO_2$. Mp 159°. Ir ν_{CeCl} 254-200br cm^{-1}.

Brezina, F., *Collect. Czech. Chem. Commun.*, 1971, **36**, 3850 (*synth, ir*)
Barry, J. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1265 (*synth, ir, uv-vis, tga*)

$C_6H_{18}ClN_4Pd^{\oplus}$

IC-005312

Chloro[tris(2-aminoethyl)amine]palladium(*II*)(1+)
[N,N-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N‴]*chloropalladium*(*1+*), *10CI*



M 288.1 (ion)
Probably mixed 4- and 5-coord. in soln.; 4-coord. in solid state as shown. Similar compds. obtd. with Br, I, NCS.

Chloride: [74735-08-3].
$C_6H_{18}Cl_2N_4Pd$ M 323.5
Light yellow solid.

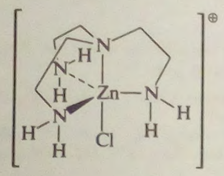
Bhattacharya, S.N. *et al, Inorg. Chim. Acta*, 1980, **41**, 67 (*synth*)

$C_6H_{18}ClN_4Zn^{\oplus}$

IC-005313

Chloro[tris(2-aminoethyl)amine]zinc(1+)
[N,N-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*chlorozinc*(*1+*), *9CI*. [*4*-(*2-Aminoethyl*)*diethylenetriamine*]*chlorozinc*(*1+*). *Chloro*(*β,β′,β″-triaminotriethylamine*)*zinc*(*1+*)

[45979-84-8]



M 247.0 (ion)

Chloride: [19356-56-0].
$C_6H_{18}Cl_2N_4Zn$ M 282.5
Cryst. +½EtOH (EtOH). Mod. sol. MeCN, $MeNO_2$, MeOH, polar solvs.; insol. $CHCl_3$, other halogenated hydrocarbons.

Perchlorate: [20037-56-3].
Cryst. (EtOH). Mod. sol. MeCN, $MeNO_2$, MeOH, polar solvs.; insol. $CHCl_3$ and other halogenated hydrocarbons.
▷ Potentially explosive.

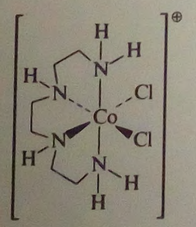
Tetraphenylborate: [20249-84-7].
Platelets (EtOH). Mod. sol. MeCN, $MeNO_2$, MeOH, polar solvs.; insol. $CHCl_3$, other halocarbons.

Interrante, L.V., *Inorg. Chem.*, 1968, **7**, 943 (*synth, ir*)
Sime, R.J. *et al, Inorg. Chem.*, 1971, **10**, 537 (*cryst struct*)
Cayley, G.R. *et al, Trans. Faraday Soc.*, 1971, **67**, 2896 (*raman*)

$C_6H_{18}Cl_2CoN_4^{\oplus}$

IC-005314

Dichloro(triethylenetetramine)cobalt(*III*)(1+)
Dichloro(*1,4,7,10-tetraazadecane*)*cobalt*(III)(*1+*)



cis-α-form

M 276.0 (ion)

cis-α-form
Chloride: Purple cryst. Sol. boiling 3*M* HCl. Has been resolved.

cis-β-form
Chloride: [15243-43-3].
Mauve (red-violet) cryst. + ½H_2O. Sol. dil. HOAc. Aquates rapidly, but has been resolved.

trans-form
Chloride: [15156-08-8].
Green cryst. + HCl + H_2O. Sol. MeOH.

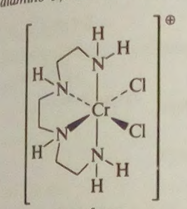
[30482-52-1, 33393-49-6]

Basolo, F., *J. Am. Chem. Soc.*, 1948, **70**, 2634 (*synth*)
Buckingham, D.A. *et al, Inorg. Chem.*, 1967, **6**, 1032 (*synth, uv-vis, pmr*)
Sargeson, A.M. *et al, Inorg. Chem.*, 1967, **6**, 787, 2172 (*synth, isomers, resoln, uv-vis, pmr, ir*)
Buckingham, D.A. *et al, J. Am. Chem. Soc.*, 1974, **96**, 1713 (*reactions*)

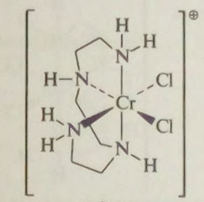
$C_6H_{18}Cl_2CrN_4^{\oplus}$

IC-005315

Dichloro(triethylenetetramine)chromium(*III*)(1+), 8CI
[N,N′-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*dichlorochromium*(*1+*), *11CI*, *10CI*, *9CI*. *Dichloro*(*1,8-diamino-3,6-diazaoctane*)*chromium*(III)



cis,α-form



cis,β-form

M 269.1 (ion)
Two isomers prepd. Presence of H_2O in solv. leads to formation of *cis* -α form. Dry solv. (MeOH) necessary to obtain *cis-β* form.

cis-α-form [46135-51-7]
Cl ligands readily replaced by SCN, azide and oxalate. λ_{max} 396, 535 nm (0.1*M* HCl).

Chloride: [14883-60-4].
Lilac powder.

Perchlorate: [15738-64-4].
Synth. from α-[Cr(trien)ox]ClO_4 + $SOCl_2$ + H_2O.
Purple cryst. (8*M* $NaClO_4$ aq.).
▷ Potentially explosive.

cis-β-form
Isom. rapidly to *cis*, α-form in presence of H_2O. λ_{max} 403, 542 nm (MeOH).

Chloride: [57793-29-0].
Purple powder. λ_{max} 402, 538 nm (reflectance).

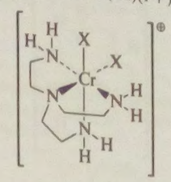
[15555-97-2, 61587-73-3, 68462-42-0]

House, D.A. *et al, J. Am. Chem. Soc.*, 1966, **88**, 2156 (*synth, ir, uv-vis*)
Garner, C.S. *et al, Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Fordyce, W.A. *et al, Inorg. Chem.*, 1977, **16**, 1154 (*synth, uv-vis, kinetics, ir*)
Thompson, M.S. *et al, Inorg. Chem.*, 1979, **18**, 1580 (*photochem*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 808 (*rev*)

$C_6H_{18}Cl_2CrN_4^{\oplus}$

IC-005316

Dichloro[tris(2-aminoethyl)amine]chromium(*III*)(1+)
[N,N-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*dichlorochromium*(*1+*), *10CI*, *9CI*. *Dichloro*(*2,2′,2″-triaminotriethylamine*)*chromium*(III)(*1+*)



X = Cl

M 269.1 (ion)
Approx. octahedral cation.

Chloride: [57718-97-5].
Synth. from $[Cr(OH_2)_4Cl_2]Cl.2H_2O$ in DMSO + ligand. Deep purple cryst.

Garner, C.S. *et al, Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Zipp, S.G. *et al, Inorg. Chem.*, 1976, **15**, 587 (*synth, kinetics, ir, uv-vis*)
Saliby, M.J. *et al, Inorg. Chem.*, 1981, **20**, 723 (*reaction*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 811 (*rev*)

$C_6H_{18}Cl_2FeN_2$

IC-005317

Dichlorobis(propylamine)iron(*II*)
Iron(II) *chloride bis(propylamine)*

$$FeCl_2(NH_2CH_2CH_2CH_3)_2\ (C_{2v})$$

M 244.9
Synth. from $FeCl_2$ + propylamine. Colourless cryst.; forms a white powder on removal of excess amine. $\mu_{eff} = 4.97\mu_B$.

McGregor, W.R. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 1027 (*synth, ir, magnetism*)

$C_6H_{18}Cl_2FeP_2$

IC-005318

Dichlorobis(trimethylphosphine)iron(*II*), 9CI

[55853-16-2]

$$FeCl_2(PMe_3)_2$$

M 278.9
Paramagnetic. Tetrahedral at Fe; numerous other phosphine analogues are known. Synth. from $FeCl_2$ + PMe_3. V. pale-green needles. Sol. THF, CH_2Cl_2, pentane. Mp 115-117°, Mp 108-112°. THF or CH_2Cl_2 solns. react with O_2 to give bright-red solns. Ir ν_{FeCl} 360 cm^{-1}.

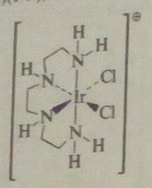
Karsch, H.H., *Chem. Ber.*, 1977, **110**, 2222 (*synth, spectra*)
Harris, T.V. *et al, J. Am. Chem. Soc.*, 1978, **100**, 6966 (*synth*)
Inorg. Synth., 1980, **20**, 70 (*synth*)

IC-005319

$C_6H_{18}Cl_2IrN_4^{\oplus}$

Dichloro(triethylenetetraamine)iridium(*III*)(1+)

[N,N′-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*dichloroiridium*(III)(*1+*), *10Cl*



M 409.3 (ion)

Tentative struct. shown.

Chloride: [72894-55-4].
Yellow solid. Sol. H_2O.

Burgess, J. *et al*, *J. Inorg. Nucl. Chem.*, 1979, **41**, 1215 (*synth, kinetics*)

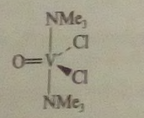
IC-005320

$C_6H_{18}Cl_3N_3OV$

Dichlorooxobis(trimethylamine)vanadium(*IV*), 8Cl

Dichlorobis(N,N-*dimethylmethanamine*)*oxovanadium*(IV), *11Cl*

[18661-54-6]



M 256.0

Trigonal bipyramid. The mono-and di-methylamine complexes are also known. Synth. by dissolving $VOCl_3$ in NMe_3 in an evacuated ampoule. Blue solid. Paramagnetic; μ_{eff} = 1.73 μ_B. Ir $\nu_{V=O}$ 990 cm^{-1}.

Baker, K.L. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1881 (*synth, ir, magnetism*)

Drake, J.E. *et al*, *J. Chem. Soc. A*, 1968, 1000 (*cryst struct*)

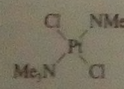
IC-005321

$C_6H_{18}Cl_2N_2Pt$

Dichlorobis(trimethylamine)platinum(*II*)

Dichlorobis(N,N-*dimethylmethanimine*)*platinum*, *9Cl*

[37106-25-5]



M 384.2

Only *trans*-isomer known. Golden-yellow plates. Sol. $CHCl_3$, $(Me)_2CO$, C_6H_6. Mp 207-208° dec.

Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1298; 1976, 459 (*synth, ir, raman, pmr, Pt-195 nmr*)

Louwen, J.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 141 (*pe*)

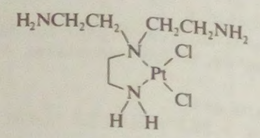
IC-005322

$C_6H_{18}Cl_2N_4Pt$

Dichloro[tris(2-aminoethyl)amine]platinum(*II*)

[N,N-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*]*dichloroplatinum*(II), *9CI*

[59538-44-2]



M 412.2

Potentially tetradentate ligand acts as bidentate. *cis*-Square planar struct.

Dihydrochloride:
$C_6H_{20}Cl_4N_4Pt$ M 485.1
Yellow cryst. (HCl). Sol. 1*M* HCl, H_2O. Mp 188° dec.

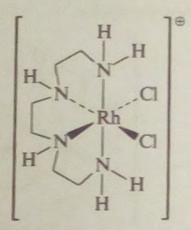
Natile, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 626.

IC-005323

$C_6H_{18}Cl_2N_4Rh^{\oplus}$

Dichloro(triethylenetetramine)rhodium(*III*)(1+)

[N,N′-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*dichlororhodium*(III)(*1+*), *9CI*



cis,α-form

M 320.0 (ion)

cis,α-form

Chloride: [42744-85-4].
Yellow solid. Sol. H_2O.

cis,β-form

Chloride: [42744-86-5].
Yellow solid. Sol. H_2O.

trans-form

Perchlorate: [42744-87-6].
Yellow cryst. Sol. H_2O.

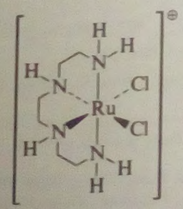
Gidney, P.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1462 (*synth, uv, kinetics, photochem*)

IC-005324

$C_6H_{18}Cl_2N_4Ru^{\ominus}$

Dichloro(triethylenetetramine)ruthenium(*III*)(1+), 8Cl

Dichloro(*1,8-diamino-3,6-diazaoctane*)*ruthenium*(III)(*1+*)



M 318.2 (ion)

Prepd. by treating Tris(oxalato)ruthenate(*III*)(3−), IC-005659 with the tetradentate ligand in 5*M* HCl. Sol. H_2O. Readily hydrated in H_2O.

Chloride: [15406-37-8].

Orange cryst. + $1H_2O$. Ir ν_{RuCl} 327, 282 cm^{-1}.

[22327-27-1]

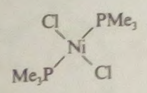
Broomhead, J.A. *et al*, *J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv*)
Broomhead, J.A. *et al*, *Inorg. Chem.*, 1968, **7**, 2519 (*hydration*)

IC-005325

$C_6H_{18}Cl_2NiP_2$

Dichlorobis(trimethylphosphine)nickel(*II*), 8Cl

[19232-05-4]



M 281.7

Prob. *trans*-sq. planar. Synth. from Nickel(*II*) chloride ($NiCl_2$), IC-016717 + PMe_3. Useful intermed. for synth. of organometallic Ni compds. by reaction with LiR or RMgCl. Dark red cryst. (EtOH). Sol. CH_2Cl_2. Mp 180-190°.

[20087-67-6, 103421-62-1]

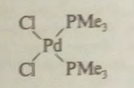
Boorman, P.M. *et al*, *Inorg. Nucl. Chem. Lett.*, 1968, **4**, 101 (*ir*)
Merle, A. *et al*, *J. Mol. Struct.*, 1972, **13**, 413 (*synth, ir, uv, raman, magnetism*)
Meier, P.M. *et al*, *Inorg. Chem.*, 1979, **18**, 610 (*uv, P-31 nmr*)
Carmona, E. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 6424 (*reaction*)

IC-005326

$C_6H_{18}Cl_2P_2Pd$

Dichlorobis(trimethylphosphine)palladium(*II*)

[25892-38-0]



cis-form

M 329.4

Ir, pmr show that a mixt. of *cis*- and *trans*-isomers exists in soln., but the solid form is predominantly *cis*; isomers have not been characterised separately, pure solid *trans*-form has not been obt. Synth. from $AgNO_3$, PMe_3 and $NaPdCl_4.3H_2O$. Greenish-yellow cryst. (MeOH). Mp 281-282° dec.

[20136-10-1, 20136-11-2]

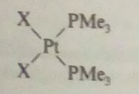
Evans, J.G. *et al*, *J. Chem. Soc. A*, 1968, 464 (*synth*)
Goodfellow, R.J. *et al*, *J. Chem. Soc. A*, 1968, 1604 (*ir*)
Duddell, D.A. *et al*, *J. Chem. Soc. A*, 1969, 2134; 1970, 545 (*ir, raman, pmr*)
Park, P.J.D. *et al*, *Spectrochim. Acta, Part A*, 1969, **25**, 909 (*ir, raman*)
Venanzi, L.M. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 62 (*uv*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 523 (*P-31 nmr*)

IC-005327

$C_6H_{18}Cl_2P_2Pt$

Dichlorobis(trimethylphosphine)platinum(*II*), 8Cl

[19471-47-7]



cis-form

X = Cl

M 418.1

Well studied example of *cis-trans* isomerism.

cis-form [15630-86-1]

trans-form [21545-76-6]

Duddell, D.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 879 (*synth, ir, raman*)
Duddell, D.A. *et al*, *J. Chem. Soc. A*, 1969, 2134 (*pmr*)
Venanzi, L.M. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 62 (*uv*)
Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 459 (*Pt-195 nmr*)
del Pra, A. *et al*, *Cryst. Struct. Commun.*, 1979, **8**, 737 (*cryst struct*)

IC-005328

$C_6H_{18}Cl_3CrN_2$

Trichlorobis(trimethylamine)chromium(*III*)

Bis(*trimethylamine*)*chromium trichloride*. *Chromium*(III) *chloride bis*(*trimethylamine*)

$CrCl_3(NMe_3)_2$

M 276.5

Trigonal pyramidal struct. with axial NMe_3. Synth. from $CrCl_3$, Zn dust and Me_3N. Purple-blue cryst. (C_6H_6). Insol. 3,3,5-trimethylpentane. μ_{eff} = 3.88μ_B (298 K).

Greene, P.T. *et al*, *J. Chem. Soc. A*, 1971, 3636 (*cryst struct*)
Duckworth, M.W. *et al*, *J. Chem. Soc. A*, 1967, 1592 (*synth, ir, uv-vis*)

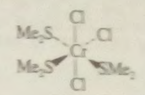
IC-005329

$C_6H_{18}Cl_3CrS_3$

Trichlorotris(dimethyl sulfide)chromium(*III*)

Trichlorotris(*methyl sulfide*)*chromium*(III), *8Cl*. *Chromium*(III) *chloride tris*(*dimethyl sulfide*)

[31363-25-4]



M 344.7

Pseudo-octahedral complex, with *mer* config. suggested by ir. Blue-violet cryst. Sol. C_5H_{12}, dimethylsulfide; insol. hexane. On recryst. in C_6H_6 forms dimeric $[CrCl_3(SMe_2)_2]_2$.

Clark, R.J.H. *et al*, *Inorg. Chim. Acta*, 1970, **4**, 533 (*synth, uv-vis, ir*)

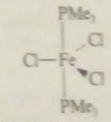
IC-005330

$C_6H_{18}Cl_3FeP_2$

Trichlorobis(trimethylphosphine)iron(*III*), 12Cl

Iron(III) *chloride bis*(*trimethylphosphine*)

[120263-16-3]



M 314.3

Trigonal bipyramidal at Fe. Synth. from PMe_3 + $FeCl_3$ in toluene. Purple cryst. (toluene/heptane). The obsd. spin equilm. ($S=\frac{1}{2}$, $S=\frac{5}{2}$) is phosphine dependent.

Walker, J.D. *et al*, *Inorg. Chem.*, 1989, **28**, 1793 (*synth, ir, uv, struct, magnetism*)

IC-005331

$C_6H_{18}Cl_3IrS_3$

Trichlorotris(dimethyl sulfide)iridium(*III*)

Trichlorotris[*thiobis*[*methane*]]*iridium*, *9CI*

[35933-29-0]

$IrCl_3(SMe_2)_3$

M 484.9

mer-Octahedral config. only. Yellow solid (EtOH). Sol. C_6H_6, EtOH.

Allen, E.A. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 613 (*synth, ir, uv, pmr*)
Williams, A.F. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1952 (*mössbauer*)

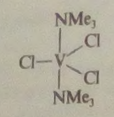
IC-005332

$C_6H_{18}Cl_3N_2V$

Trichlorobis(trimethylamine)vanadium(*III*), 8CI

Trichlorobis(N,N-*dimethylmethanamine*)*vanadium*(III), *11CI. Vanadium*(III) *chloride bis*(*trimethylamine*)

[20538-61-8]



M 275.5
Trigonal bipyramidal, may consist of more than one ax/eq. isomer. Synth. either by reducing VCl_4 with excess Me_3N in a sealed tube or by direct reaction of VCl_3 with NMe_3 at 100° in a sealed tube. Light mauve solid, v. sensitive to O_2 and H_2O. Sol. C_6H_6. Subl. 100°. Paramagnetic, $\mu_{eff} = 2.69\mu_B$ (291K).

[19631-72-2]

Fowles, G.W.A. *et al, J. Chem. Soc. A*, 1967, 1592 (*synth, ir, uv-vis, magnetism*)
Crouch, P.C. *et al, J. Chem. Soc. A*, 1968, 2172 (*uv-vis*)
Greene, P.T. *et al, J. Chem. Soc. A*, 1969, 1621 (*cryst struct*)
Kiesel, R. *et al, Inorg. Chem.*, 1973, **12**, 1090 (*synth*)

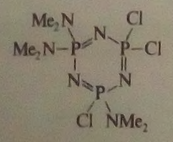
IC-005333

$C_6H_{18}Cl_3N_6P_3$

2,2,4-Trichloro-4,6,6-tris(dimethylamino)-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 9CI

2,2,4-Trichloro-4,6,6-tris(dimethylamino)-2,2,4,4,6,6-hexahydrocyclotriphosphazene. 2,2,4-Trichloro-4,6,6-tris(dimethylamino)-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2,4-Trichloro-4,6,6-tris(dimethylamino)-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine

[957-07-3]



M 373.5
Cryst. (pentane). Mp 71°.

Keat, R. *et al, J. Chem. Soc.*, 1965, 2215 (*synth, struct, pmr*)
Strahlberg, R. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 2005 (*ir, raman*)
Keat, R. *et al, J. Chem. Soc. A*, 1968, 703 (*pmr*)
Ahmed, F.R. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 513 (*cryst struct*)
Keat, R. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1648 (*nqr*)
Green, B. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1042 (*pe*)
Dagliesh, W.H. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 309 (*nqr*)
Faucher, J.-P. *et al, J. Mol. Struct.*, 1975, **25**, 109 (*struct*)
Keat, R. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1582 (*P-31 nmr*)
Katti, K.V. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 285 (*glc*)
Grunditz, N. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 925 (*props*)

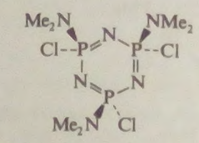
$C_6H_{18}Cl_3N_6P_3$

IC-005334

2,4,6-Trichloro-2,4,6-tris(dimethylamino)-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine

2,4,6-Trichloro-2,4,6-tris(dimethylamino)-2,2,4,4,6,6-hexahydrocyclotriphosphazene. 2,4,6-Trichloro-2,4,6-tris(dimethylamino)-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,4,6-Trichloro-2,4,6-tris(dimethylamino)-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine

[3721-13-9]



(2α,4α,6α)-*form*

M 373.5
Cis- and *trans*-forms equilibrate in presence of $AlCl_3$.

(2α,4α,6α)-*form* [1216-69-9]
cis-*form*
Solid. Mp 152°.

(2α,4α,6β)-*form* [957-10-8]
trans-*form*
Cryst. (pet. ether). Mp 105°.

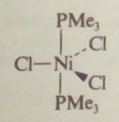
Keat, R. *et al, J. Chem. Soc.*, 1965, 2215 (*synth, struct, pmr*)
Strahlberg, R. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 2005 (*ir, raman*)
Keat, R. *et al, J. Chem. Soc. A*, 1968, 703 (*pmr*)
Ahmed, F.R. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 3530; 1975, **31**, 1028 (*cryst struct*)
Green, B. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1042 (*pe*)
Dagleish, W.H. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 309 (*nqr*)
Nabi, S.N. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 588 (*synth*)
Keat, R. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1582 (*P-31 nmr*)
Connelly, A. *et al, J. Magn. Reson.*, 1978, **30**, 439 (*nqr*)
Katti, K.V. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 285 (*glc*)
Gremditz, N. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 925 (*props*)

IC-005335

$C_6H_{18}Cl_3NiP_2$

Trichlorobis(trimethylphosphine)nickel(*III*), 11Cl

[90738-93-5]



M 317.2
Prob. trigonal bipyramidal struct. with *trans*-PMe_3. Most stable $Ni(PR_3)_2Cl_3$ complex. Synth. from Dichlorobis(trimethylphosphine)nickel(*II*), IC-005325 + NOCl in CH_2Cl_2 at −78°. Purple-red solid. Br analogue known. Paramagnetic.

Higgins, S.J. *et al, Inorg. Chim. Acta*, 1984, **84**, 1 (*synth, ir, uv, esr*)

IC-005336

$C_6H_{18}Cl_3O_3OsS_3$

Trichlorotris(dimethylsulfoxide)osmium(*III*)

Trichlorobis[*sulfinylbis*[*methane*]-O][*sulfinylbis*[*methane*]-S]*osmium*(III)

[66009-49-2]

$$OsCl_3(O{=}SMe_2)_3$$

M 530.9
Synth. by heating H_2OsCl_6 in DMSO.

Antonov, P.G. *et al, Zh. Neorg. Khim.*, 1978, **23**, 441 (*synth, ir, pmr*)

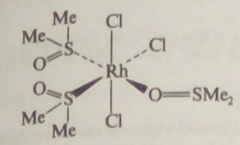
IC-005337

$C_6H_{18}Cl_3O_3RhS_3$

Trichlorotris(dimethyl sulfoxide)rhodium(*III*)

Trichloro[*sulfinylbis*[*methane*]-O]*bis*[*sulfinylbis*[*methane*]-S]*rhodium*(III), *9CI*

[56195-04-1]



M 443.6
Orange cryst. Sol. H_2O. *mer*-Config. only known. Two of the DMSO molecules coordinate to Rh through S and one through O.

Kukushkin, Y.N. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 1115 (*synth, uv, ir*)
Sokol, V.I. *et al, Koord. Khim.*, 1975, **1**, 577 (*cryst struct*)

IC-005338

$C_6H_{18}Cl_3O_3RuS_3^{\ominus}$

Trichlorotris(dimethyl sulfoxide)ruthenate(*II*)(1−)

Trichlorotris[*sulfinylbis*[*methane*]-S]*ruthenate*(*1−*), *9CI*

$$RuCl_3[S(O)Me_2]_3^{\ominus}$$

M 441.8 (ion)
fac-Octahedral isomer; all DMSO ligands are *S*-bonded, is the principal form; other isomers are known. Prepd. by reducing '$RuCl_3.xH_2O$' in DMA with H_2 in the presence of DMSO; the solvent gives rise to the $[NMe_2H_2]^{\oplus}$ cation. Sol. DMSO, DMA, H_2O. Ir ν_{RuCl} 265, 241 cm^{-1}.

Me_2NH_2 salt: [57077-65-3].
Yellow cryst. Mp 195° dec. Ir ν_{SO} 1100 cm^{-1}. Ru—S 226.1; Ru—Cl 242.6; S—O 148 pm.

McMillan, R.S. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1006 (*synth, cryst struct, ir, pmr, uv, catalysis*)
James, B.R. *et al, J. Mol. Catal.*, 1975/76, **1**, 439 (*catalysis*)
Barnes, J.R. *et al, J. Chem. Res.* (*S*), 1979, 350; *J. Chem. Res.* (*M*), 1979, 4301 (*synth, pmr, ir*)

IC-005339

$C_6H_{18}Cl_3O_3RuS_3$

Trichlorotris(dimethyl sulfoxide)ruthenium(*III*)

Trichlorotris[*sulfinylbis*[*methane*]-O]*ruthenium*(III), *9CI. Ruthenium*(III) *chloride tris*(*dimethyl sulfoxide*)

[65982-39-0]

$$RuCl_3(O{=}SMe_2)_3$$

M 441.8
Thought to be *fac*-octahedral with *O*-bonded sulfoxides. Red or yellow solid. Mp 108°. $\mu_{eff} = 1.6\mu_B$; Ir ν_{RuCl} 324 cm^{-1}.

[76647-72-8]

Gilbert, J.D. *et al, J. Chem. Soc. A*, 1968, 2198 (*synth, ir, magnetism*)
Antonov, P.G. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 245 (*synth, ir*)

IC-005340

$C_6H_{18}Cl_3O_3S_3Y$

Trichlorotris(dimethyl sulfoxide)yttrium(*III*)

Trichlorotris[*sulfinylbis*[*methane*]-O]*yttrium*(III). *Yttrium*(III) *chloride tris*(*dimethyl sulfoxide*)

[15657-46-2]

$$YCl_3(O{=}SMe_2)_3$$

M 429.6
Presumed 6-coordinate. Hygroscopic white cryst. Sol. MeOH, MeCN, DMF, DMSO. Mp 121°. Non electrolyte in MeCN.

Ramalingam, S.K. *et al, Curr. Sci.*, 1966, **35**, 233 (*synth, ir*)
Ramalingam, S.K. *et al, Z. Anorg. Allg. Chem.*, 1967, **353**, 216.
Golub, A.M. *et al, Uzb. Khim. Zh.*, 1977, **43**, 1281; *CA*, **86**, 146625 (*synth*)

IC-005341

$C_6H_{18}Cl_3O_3Ti$

Trichlorotris(ethanol)titanium(*III*), 11Cl

Trichlorotris(*ethyl alcohol*)*titanium*, *8CI. Titanium*(III) *chloride tris*(*ethanol*)

[30669-31-9]

$$(EtOH)_3TiCl_3$$

M 292.4
Synth. either by dissolving $TiCl_3$ in EtOH or by photoreduction of $TiCl_4$ in EtOH by sunlight. Blue-green solid. Forms EtOH solvate.

[86420-50-0]

Hunt, M.R. *et al, Inorg. Nucl. Chem. Lett.*, 1970, **6**, 529 (*photochem synth*)
Zikmund, M. *et al, Chem. Zvesti*, 1979, **33**, 206 (*thermal anal*)
Kuchmii, S.Ya. *et al, Koord. Khim.*, 1984, **10**, 1505; *CA*, **102**, 71612m (*synth, uv-vis, esr, deriv*)

IC-005342

$C_6H_{18}Cl_3RhS_3$

Trichlorotris(dimethyl sulfide)rhodium(*III*)

Trichlorotris[*thiobis*[*methane*]]*rhodium*(III), *9CI*

[29201-22-7]

$$RhCl_3(SMe_2)_3$$

M 395.6
Config. not specified. Orange-red cryst. Sol. C_6H_6.

Allen, E.A. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 613 (*synth, ir, pmr*)

IC-005343

$C_6H_{18}Cl_3RuS_3$

Trichlorotris(dimethyl sulfide)ruthenium(*III*)

Trichlorotris[*thiobis*[*methane*]]*ruthenium*(III), *9CI. Ruthenium*(III) *chloride tris*(*dimethyl sulfide*)

[32648-21-8]

$$RuCl_3(SMe_2)_3$$

M 393.8
Isomeric form unknown. Prepd. by treating ethanolic $RuCl_3.xH_2O$ with SMe_2. Red solid. Mp 120° dec. $\mu_{eff} = 2.1\mu_B$.

[61688-28-6]

Chatt, J. *et al, J. Chem. Soc. A*, 1969, 854; 1971, 1380 (*synth, magnetism*)
Bora, T. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 1815 (*synth, ir*)
Contreras, R. *et al, J. Organomet. Chem.*, 1979, **179**, C55 (*electrochem*)

IC-005344

$C_6H_{18}Cl_4IrP_2$

Tetrachlorobis(trimethylphosphine)iridium(*IV*), 9CI

[42750-88-9]

$$IrCl_4(PMe_3)_2$$

M 486.1
trans-Octahedral geometry. Pink cryst.

Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1489 (*synth, ir, raman*)

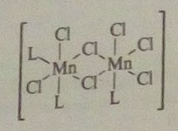
IC-005345

$C_6H_{18}Cl_4Mn_2O_3$

Di-μ-chlorodichlorotris(ethanol)dimanganese, 9Cl

Manganese dichloride compd. with ethanol (2:3). Manganese chloride ethanol ($Mn_2Cl_4.3EtOH$)

[38893-84-4]



L = EtOH

Manganese environment

M 389.8

Polymeric struct. Prepd. from $MnCl_2$ and anhyd. EtOH. Pale pink cryst.

L'Haridon, P. *et al, Rev. Chim. Minér.*, 1971, **8**, 813 (*synth, thermal dec.*)

L'Haridon, P. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 2743 (*synth, struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 30 (*rev, bibl*)

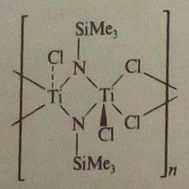
IC-005346

$C_6H_{18}Cl_4N_2Si_2Ti_2$

***catena*-Di-μ-chlorobis(μ-trimethylsilylimido) bis[chlorotitanium(*IV*)]**

Tetrachlorobis[μ-[1,1,1-trimethylsilanaminato(2−)]] dititanium, 11Cl

[55290-50-1]



M 411.9

Distorted tbp polymer. Synth. from $TiCl_4$ and 2 $NaN(SiMe_3)_2$ in THF/C_6H_6. Alternatively from $TiCl_4$ and tris(trimethylsilyl)amine. Orange solid. Sol. Et_2O, THF/C_6H_6.

Pierce-Butler, M. *et al, J. Organomet. Chem.*, 1973, **54**, C19 (*synth*)

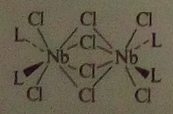
Alcock, N.W. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 627 (*cryst struct, synth*)

Vasisht, S.K. *et al, Indian J. Chem., Sect. A*, 1985, **24**, 37 (*synth, ir, pmr*)

IC-005347

$C_6H_{18}Cl_4NbP_2$

Tetrachlorobis(trimethylphosphine)niobium(*IV*)



dimer, L = PMe_3

M 386.8

Dimeric. Cf. monomeric struct. of Tetrachlorobis(triethylphosphine)niobium(*IV*), IC-008039.

Dimer: [92125-99-0]. *Tetra-μ-chlorotetrachlorotetrakis(trimethylphosphine) diniobium*(IV), *11Cl. Tetra-μ-chlorobis[dichlorobis(trimethylphosphine)niobium*(IV)] $C_{12}H_{36}Cl_8Nb_2P_4$ M 773.7

Synth. from $NbCl_4.2THF + PMe_3$ in CH_2Cl_2. Red cryst.

Manzer, L., *Inorg. Chem.*, 1977, **16**, 525 (*synth*)

Cotton, F.A. *et al, Inorg. Chem.*, 1984, **23**, 3592 (*cryst struct*)

IC-005348

$C_6H_{18}Cl_4NpO_2P_2$

Tetrachlorobis(trimethylphosphine oxide)neptunium(*IV*)

Neptunium(IV) *chloride bis(trimethylphosphine oxide)*

[104759-73-1]

$NpCl_4(O{=}PMe_3)_2$

M 563.0

Presumed 6-coordinate. Buff brown solid.

[41333-62-4]

Al-Kazzaz, Z.M.S. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 1493 (*synth, ir*)

Bagnall, K.W. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 783 (*use*)

IC-005349

$C_6H_{18}Cl_4NpO_3S_3$

Tetrachlorotris(dimethyl sulfoxide)neptunium(*IV*)

Tetrachlorotris[sulfinylbis[methane]-O]neptunium(IV). *Neptunium*(IV) *chloride tris(dimethyl sulfoxide)*

[19403-46-4]

$NpCl_4(O{=}SMe_2)_3$

M 613.2

Pink solid. Sol. hot $MeNO_2$. Unstable $NpCl_4.5DMSO$ also exists.

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 465 (*synth, ir*)

IC-005350

$C_6H_{18}Cl_4O_2P_2Th$

Tetrachlorobis(trimethylphosphine oxide)thorium(*IV*)

Thorium(IV) *chloride bis(trimethylphosphine oxide)*

[58057-89-9]

$ThCl_4(O{=}PMe_3)_2$

M 558.0

White cryst. Sl. sol. THF. Mp 39° dec.

Wassef, M.A., *Indian J. Chem.*, 1975, **13**, 1203 (*synth, ir*)

IC-005351

$C_6H_{18}Cl_4O_2P_2U$

Tetrachlorobis(trimethylphosphine oxide)uranium(*IV*)

[41333-61-3]

$UCl_4(O{=}PMe_3)_2$

M 563.9

Prob. 6-coordinate. V. hygroscopic pale green cryst. Sol. THF. Exists in two cryst. structs., α-form from THF, β-form by heating $UCl_4(Me_3PO)_6$ or $UCl_4(Me_3PO)_2$ to over 100° *in vacuo*.

Gans, P. *et al, J. Chem. Soc.*, 1964, 4172 (*synth*)

Al-Kazzaz, Z.M.S. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 1493 (*synth, ir*)

Du Preez, J.G.H. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1062 (*synth*)

IC-005352

$C_6H_{18}Cl_4O_3PaS_3$

Tetrachlorotris(dimethyl sulfoxide)protactinium(*IV*)

Protactinium(IV) *chloride tris(dimethyl sulfoxide)*

[19403-40-8]

$PaCl_4(O{=}SMe_2)_3$

M 607.2

Bright yellow solid. Oxidizes on keeping in dry Ar over 1-2 days.

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 465 (*synth, ir*)

IC-005353

$C_6H_{18}Cl_4O_3PuS_3$

Tetrachlorotris(dimethylsulfoxide)plutonium(*IV*)

Plutonium(IV) *chloride tris(dimethyl sulfoxide)*

[12079-10-6]

$PuCl_4(O{=}SMe_2)_3$

M 615.2

Red solid. Sol. hot $MeNO_2$, MeCN.

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 465 (*synth, ir*)

Alvey, J.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2326 (*use*)

IC-005354

$C_6H_{18}Cl_4O_3S_3Th$

Tetrachlorotris(dimethyl sulfoxide)thorium(*IV*)

Tetrachlorotris[sulfinylbis[methane]-O]thorium(IV)

$ThCl_4(O{=}SMe_2)_3$

M 608.2

Solid state formulation by analogy with corresp. U compd., Tetrachlorotris(dimethyl sulfoxide)uranium(*IV*), IC-005355.

Solid state-form

Dichlorohexakis(dimethyl sulfoxide)thorium(IV) *hexachlorothorate*(IV).

Dichlorohexakis[sulfinylbis[methane]-O]thorium(IV)(2+) *hexachlorothorate*(IV)(2−) $[(Me_2SO)_6ThCl_2]^{2\oplus}[ThCl_6]^{2\ominus}$. White solid. Sol. MeCN, $MeNO_2$.

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 465 (*synth, ir*)

IC-005355

$C_6H_{18}Cl_4O_3S_3U$

Tetrachlorotris(dimethyl sulfoxide)uranium(*IV*)

Tetrachlorotris[sulfinylbis[methane]-O]uranium(IV), *9Cl, 8Cl*

[12079-11-7]

$UCl_4(O{=}SMe_2)_3$

M 614.2

Possesses ionic struct. in solid state, with dodecahedral cation and octahedral anion. Can be synth. from 7:1 and 5:1 complexes on recryst. or on pumping. Exhibits complex ionisation in polar solvs. Non-electrolyte in $MeNO_2$, monomeric in MeCN.

Solid state-form: [55915-03-2]. *Dichlorohexakis(dimethyl sulfoxide)uranium*(IV) *hexachlorouranate*(IV). *Dichlorohexakis[sulfinylbis[methane]-O]uranium*(2+) *hexachlorouranate*(2−), *9Cl*

$C_{12}H_{36}Cl_8O_6S_6U_2$ M 1228.4

Grey-green cryst. Sol. MeCN, $MeNO_2$, hot Me_2CO. Mp 180-182°. See also Dichlorohexakis(dimethyl sulfoxide) uranium(*IV*)(2+), IC-008222.

[58693-89-3]

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1966, 737; 1968, 465 (*synth, ir*)

Alvey, P.J. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2308 (*ir, uv*)

du Preez, J.G.H. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 1795 (*soln props*)

Miyake, C. *et al, Chem. Phys. Lett.*, 1975, **36**, 158 (*pe*)

Bombieri, G. *et al, J. Chem. Soc., Chem. Commun.*, 1975, 188 (*cryst struct*)

Sakurai, H. *et al, J. Inorg. Nucl. Chem.*, 1980, **42**, 67 (*magnetism*)

Kumar, N. *et al, Inorg. Chim. Acta*, 1984, **95**, 211 (*synth, ir*)

IC-005356

$C_6H_{18}Cl_4O_6OsP_2$

Tetrachlorobis(trimethyl phosphite)osmium(*IV*)

Osmium(IV) *chloride bis(trimethyl phosphite)*

[61805-71-8]

$OsCl_4[P(OMe)_3]_2$

M 580.1

trans-Octahedral. Synth. from Zn/Hg and $Na_2[OsCl_6]$ in a soln. of THF and $P(OMe)_3$. Yellow powder. Sol. THF. Mp > 300°. Starting material for $Os[P(OMe)_3]_5$.

English, A.D. *et al, J. Am. Chem. Soc.*, 1977, **99**, 117 (*synth, use*)

IC-005357

$C_6H_{18}Cl_4PdSb_2$

Tetrachlorobis(trimethylstibine)palladium(*IV*)

Palladium(IV) *chloride bis(trimethylstibine)*

$PdCl_4(SbMe_3)_2$

M 581.9

Probably formed from $Cl_2 + PdCl_2(SbMe_3)_2$, but not isol.

Gulliver, D.J. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 1895.

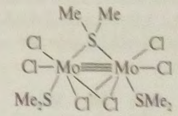
IC-005358

$C_6H_{18}Cl_6Mo_2S_3$

Di-μ-chlorotetrachloro-μ-(dimethyl sulfide)bis(dimethyl sulfide)dimolybdenum(*III*)

Di-μ-chlorotetrachloro[μ-[thiobis[methane]]] bis[thiobis[methane]]dimolybdenum(III), *11Cl*

[83789-82-6]



M 591.0

First example of a dinuclear molybdenum complex containing a bridging simple dialkyl sulfide ligand. Isomers exist. Interatomic distance, Mo—Mo 246.2 pm. Diamagnetic.

Boorman, P.M. *et al, J. Chem. Soc., Chem. Commun.*, 1982, 899 (*cryst struct, synth*)

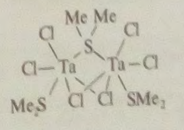
IC-005359

$C_6H_{18}Cl_6S_3Ta_2$

Hexachlorotris(dimethyl sulfide)ditantalum(*III*)

Di-μ-chlorotetrachloro-μ-(dimethyl sulfide)bis(dimethyl sulfide)ditantalum(III). *Di-(μ-chloro)(μ-dimethyl sulfide) bis[dichloro(dimethyl sulfide)tantalum*(III)]. *Di-μ-chlorotetrachloro[μ-[thiobis[methane]]]bis[thiobis[methane]] ditantalum*(III), *11Cl*

[77827-59-9]



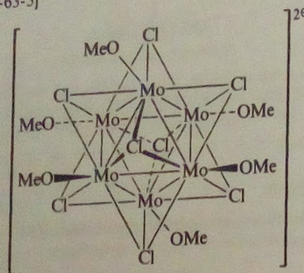
M 761.0

Bioctahedral struct. Synth. by adding Me_2S to a suspension of $TaCl_5$ in toluene, followed by 2 equivs. of Na/Hg. Starting material. Brown cryst. Sol. toluene.

Cotton, F.A. *et al, Inorg. Chem.*, 1981, **20**, 2716 (*synth, cryst struct, ir*)
Canich, J.A.M. *et al, Polyhedron*, 1986, **5**, 895 (*reactions*)

IC-005360

$C_6H_{18}Cl_8Mo_6O_6^{2\ominus}$
Octa-μ_3-chlorohexamethoxyhexamolybdate(2−), 11CI
Octakis(μ_3-chloro)hexakis(methoxymolybdate)
[88983-63-5]



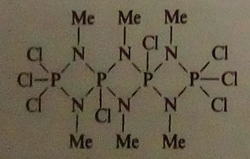
M 1045.4 (ion)
Cluster of 6 Mo atoms in an octahedral arrangement within a cube of triply-bridging Cl ligands. Each Mo has a terminal OMe ligand bound to it.

Di-Na salt: [91408-94-5]. *Molybdenum sodium chloride methoxide* ($Mo_6Na_2Cl_8(OMe)_6$)
Moisture-sensitive yellow cryst. + 10MeOH.

Chisholm, M.H. *et al, Polyhedron*, 1984, **13**, 475 (*cryst struct*)
Nannelli, P. *et al, Inorg. Chem.*, 1968, **7**, 2423 (*synth, ir, pmr*)

IC-005361

$C_6H_{18}Cl_8N_6P_4$
2,2,2,4,6,8,8,8-Octachloro-2,2,8,8-tetrahydro-1,3,5,7,9,10-hexamethyl-1,3,5,7,9,10-hexaaza-2,4,6,8-tetraphospha(P^V)dispiro[3.1.3.1]decane
[6041-62-9]



M 581.7
Synth. from PCl_5 + $[MeNH_3]Cl$. Cryst. (C_6H_6). Mp 395° dec.

Becke-Goehring, M. *et al, Z. Anorg. Allg. Chem.*, 1966, **343**, 154 (*synth*)
Weiss, J. *et al, Z. Anorg. Allg. Chem.*, 1967, **351**, 152 (*cryst struct*)
Latscha, H.P., *Z. Naturforsch., B*, 1968, **23**, 139 (*P-31 nmr*)

IC-005362

$C_6H_{18}CoN_2O_2P_2^{2\oplus}$
Dinitrosylbis(trimethylphosphine)cobalt(2+), 11CI

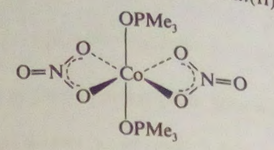
$[Co(NO)_2(PMe_3)_2]^{2\oplus}$

M 271.1 (ion)
Bis-tetraphenylborate: [101011-33-0].
Brown solid.
Tetrathiocyanatocobaltate(2−): [101011-32-9].
Green needles.

Alnaji, O. *et al, Inorg. Chem.*, 1986, **25**, 1383 (*synth, ir*)

IC-005363

$C_6H_{18}CoN_2O_8P_2$
Bis(nitrato-*O,O′*)bis(trimethylphosphine oxide)cobalt(*II*)
Bis(trimethylphosphine oxide)dinitratocobalt(II)

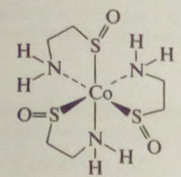


M 367.0
Octahedral complex with bidentate nitrates. Purple cryst.

Cotton, F.A. *et al, J. Am. Chem. Soc.*, 1963, **85**, 2402 (*synth, cryst struct*)

IC-005364

$C_6H_{18}CoN_3O_3S_3$
Tris[(2-aminoethyl)sulfinyl-*N,S*]cobalt(*III*), 10CI
Tris(2-aminoethanesulfenato)cobalt(III)
[73746-32-4]

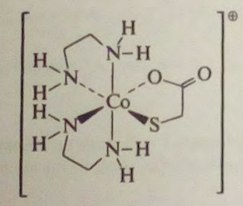


M 335.3
Octahedral. Orange-red cryst. Sol. H_2O.

Kita, M. *et al, Chem. Lett.*, 1980, 275 (*synth, uv*)
Kita, M. *et al, Bull. Chem. Soc. Jpn.*, 1981, **54**, 2995 (*cryst struct*)

IC-005365

$C_6H_{18}CoN_4O_2S^{\oplus}$
Bis(ethylenediamine)(mercaptoacetato-*O,S*)cobalt(*III*)(1+), 8CI



M 269.2 (ion)
Perchlorate: [26743-67-9].
$C_6H_{18}ClCoN_4O_6S$ M 368.6
▷ Potentially explosive.

Lane, R.H. *et al, J. Am. Chem. Soc.*, 1970, **92**, 1089 (*synth, ir*)

IC-005366

$C_6H_{18}CoN_4O_5^{\oplus}$
Aquabis(ethylenediamine)oxalatocobalt(*III*)(1+)

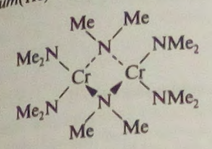
$[Co(H_2NCH_2CH_2NH_2)_2(OH_2)(C_2O_4)]^{\oplus}$

M 285.1 (ion)
Prob. monodentate oxalate. Cation prep. in aq. soln., not isol.

Chan, S.C. *et al, Inorg. Chem.*, 1971, **10**, 1317 (*synth, uv, kinetics*)

IC-005367

$C_6H_{18}CrN_3$
Tris(dimethylamido)chromium(*III*)
Chromium(III) *dimethylamide*



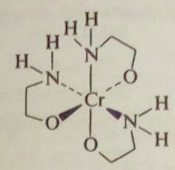
dimer

M 184.2
Dimeric cf. monomeric Tris(diisopropylamido) chromium(*III*), IC-010100.
Dimer: Bis[μ-(dimethylamido)]tetrakis(dimethylamido) dichromium
$C_{12}H_{36}Cr_2N_6$ M 368.4

Basi, J.S. *et al, J. Chem. Soc. A*, 1971, 1433.
Bradley, D.C. *et al, Acc. Chem. Res.*, 1976, **9**, 273.

IC-005368

$C_6H_{18}CrN_3O_3$
Tris(2-aminoethanolato)chromium(*III*)
[38819-71-5]

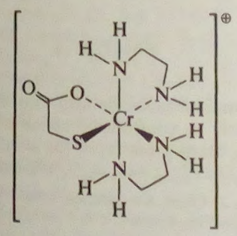


M 232.2
Obt. as trihydrate. Presumed octahedral but struct. not descr.
Trihydrate: [17438-91-4].
Synth. from $CrCl_3$, $H_2NCH_2CH_2OH$ and H_2O. Cryst. Attempted dehydration causes dec.

Kolosci, L. *et al, Inorg. Chem.*, 1983, **22**, 3053 (*synth, uv, deriv*)

IC-005369

$C_6H_{18}CrN_4O_2S^{\oplus}$
Bis(ethylenediamine)[2-mercaptoacetato(2−)-*O,S*] chromium(*III*)(1+)
Bis(1,2-ethanediamine-N,N′)[mercaptoacetato(2−)-O,S] chromium(III)(*1+*), *10CI, 9CI*
[41654-60-8]

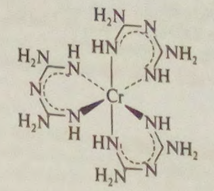


M 262.2 (ion)
Pseudooctahedral complex.
Perchlorate: [41212-24-2].
Cherry-red cryst. (H_2O).

Weschler, C.J. *et al, Inorg. Chem.*, 1973, **12**, 2682 (*synth, aquation, uv-vis*)
Elder, R.C. *et al, Inorg. Chem.*, 1973, **12**, 2690 (*cryst struct*)

IC-005370

$C_6H_{18}CrN_{15}$
Tris(biguanidato)chromium(*III*)
Tris(imidodicarbonimidic diamidato-N″,N‴)chromium(III), *9CI*
[59136-96-8]



M 352.3
Octahedral at Cr. Orange-red cryst. + $1H_2O$.

Coghi, L. *et al, Acta Crystallogr., Sect. B*, 1976, **32**, 842 (*cryst struct, synth*)

IC-005371

$C_6H_{18}DyN_3O_{12}S_3$
Tris(dimethyl sulfoxide)tris(nitrato)dysprosium(*III*)
Tris(nitrato-O,O′)tris[sulfinylbis[methane]-O]dysprosium(III), *11CI. Dysprosium*(III) *nitrate tris(dimethyl sulfoxide)*
[97057-48-2]

$Dy(NO_3)_3(O{=}SMe_2)_3$

M 582.9
Probably 9-coordinate with bidentate nitrates. Yellow cryst. Sol. MeCN, Me_2CO, MeOH, DMSO.
[99455-84-2]

Su, Q. *et al, Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581 (*synth*)
Bao, F. *et al, Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

IC-005372

$C_6H_{18}ErN_3O_{12}S_3$
Tris(dimethyl sulfoxide)tris(nitrato)erbium(*III*)
Tris(nitrato-O,O′)tris[sulfinylbis[methane]-O]erbium(III). *Erbium*(III) *nitrate tris(dimethyl sulfoxide)*
[36606-61-8]

$Er(NO_3)_3(O{=}SMe_2)_3$

M 587.6
9-Coordinate, with all nitrates bidentate. Pink cryst. Sol. MeCN, Me_2CO, MeOH, DMSO.

Aslanov, L.A. *et al, J. Struct. Chem. USSR* (*Engl. Transl.*), 1972, **13**, 1021 (*cryst struct*)
Kawano, Y. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 701 (*ir, raman*)
Su, Q. *et al, Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581.
Bao, F. *et al, Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir*)

IC-005373

$C_6H_{18}FeN_2O_8P_2$
Dinitrosylbis(trimethyl phosphite-*P*)iron, 9CI
Dinitrosylbis(phosphorous acid)iron hexamethyl ester, 8CI
[23131-33-1]

$[(MeO)_3P]_2Fe(NO)_2$

M 364.0
Red liq. Sol. common org. solvs. Mp −42°. Dec. at 119°. Stable in air at r.t. ca. 1 hr., dec. after 1 week at −30° under N_2.

Kruck, T. *et al, Z. Anorg. Allg. Chem.*, 1973, **402**, 16 (*synth, ir, ms*)

IC-005374

$C_6H_{18}FeO_6^{3\ominus}$

Hexamethoxyferrate(*III*)(3−)

$[Fe(OMe)_6]^{3\ominus}$ (O_h)

M 242.0 (ion)

Tri-K salt: [15021-89-3].
Synth. from KOMe + $FeCl_3$ in MeOH, followed by freeze drying. Red-brown solid.

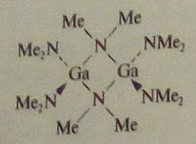
Ludman, C.J. *et al, J. Chem. Soc. A*, 1966, 1816 (*synth*)

IC-005375

$C_6H_{18}GaN_3$

Tris(dimethylamido)gallium

Tris(dimethylamino)gallane



Dimer

M 201.9
Dimeric.

Dimer: [57731-40-5]. *Bis[μ-(N-methylmethanaminato)]tetrakis(N-methylmethanaminato)digallium, 9CI*
$C_{12}H_{36}Ga_2N_6$ M 403.9
Colourless air and moisture sensitive cryst. (pentane). Mp 90-92°. Dec. at 120-130°/10^{-2} mm.

Nöth, H. *et al, Z. Naturforsch., B*, 1975, **30**, 681 (*synth, pmr, ir*)
Waggoner, K.M. *et al, Polyhedron*, 1990, **9**, 257 (*synth, cryst struct*)

IC-005376

$C_6H_{18}GeO_2Si_2$

Bis(trimethylsilyloxy)germanium

$Ge(OSiMe_3)_2$

M 250.9
Golden oil. Sol. pentane, toluene, THF.

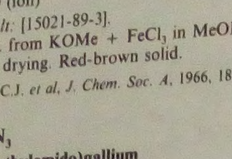
DuMont, W.W. *et al, Chem. Ber.*, 1981, **114**, 1180.

IC-005377

$C_6H_{18}Hg_3S_6^{2\ominus}$

Hexakis(methylthio)dimercurate(2−)

Bis[μ-(methanethiolato)]tetrakis(methanethiolato)dimercurate(2−)



M 683.7 (ion)
Some dissoc. of dianion in EtOH soln. to $[Hg(SMe)_3]^{\ominus}$.

Bis-Et_4N salt: [93239-67-9].
Cryst. (aq. EtOH). Sol. Py. Mp 77-78°.

Bowmaker, G.A. *et al, Aust. J. Chem.*, 1984, **37**, 1607 (*synth, cryst struct, ir, raman*)

IC-005378

$C_6H_{18}HoN_3O_{12}S_3$

Tris(dimethyl sulfoxide)tris(nitrato)holmium(*III*)

Tris(nitrato-O,O′)tris[sulfinylbis[methane]-O]holmium(III). Holmium(III) nitrate tris(dimethyl sulfoxide)

[19631-11-9]

$Ho(NO_3)_3(O{=}SMe_2)_3$

M 585.3
Probably 9-coordinate with bidentate nitrates. Yellow cryst. Sol. MeCN, MeOH, Me_2CO, DMSO. Mp 155°.

Ramalingam, S.K. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth, ir*)

IC-005379

$C_6H_{18}I_2NiP_2$

Diiodobis(trimethylphosphine)nickel(*II*)

[70252-69-6]

$NiI_2(PMe_3)_2$

M 464.6
Isol. of this compd. not confirmed. Dark brown solid. Reacts with CO, forming $Ni(CO)I_2(PMe_3)_2$. Diamagnetic.

Beg, M.A.A. *et al, Can. J. Chem.*, 1961, **39**, 595 (*synth, uv-vis, magnetism*)
Saint-Joly, C. *et al, Adv. Chem. Ser.*, 1979, **173**, 152 (*reactions*)

IC-005380

$C_6H_{18}I_2P_2Pt$

Diiodobis(trimethylphosphine)platinum(*II*), 8CI

[19471-49-9]

As Dichlorobis(trimethylphosphine)platinum(*II*), IC-005327 with

X = I

M 601.0
Well studied example of *cis-trans* isomerism.

cis-form [21258-95-7]
Yellow solid. Sol. CH_2Cl_2.

trans-form [15703-03-4]
More sol. than *cis*-isomer. Yellow solid. Sol. CH_2Cl_2.

Duddell, D.A. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 879 (*synth, ir, raman*)
Duddell, D.A. *et al, J. Chem. Soc. A*, 1969, 2134 (*pmr*)
Clark, D.T. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 602 (*pe*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 459 (*Pt-195 nmr*)
Hitchcock, P.D. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2038 (*cryst struct*)
Hitchcock, P.D. *et al, J. Organomet. Chem.*, 1977, **133**, 273 (*cryst struct*)

IC-005381

$C_6H_{18}I_3MnP_2$

Triiodobis(trimethylphosphine)manganese(*III*), 11CI

[91924-71-9]

$MnI_3(PMe_3)_2$

M 587.8
Trigonal bipyramidal molecule with axial P; Mn—P 243-244 pm. Synth. by controlled reaction of O_2 with $MnI_2(PMe_3)$. Dark green cryst. (by subl.). $Subl._{0.1}$ 120°. $\mu_{eff} = 4.8\mu_B$. Ir ν_{Mn-P} 445; ν_{Mn-I} 192 cm^{-1}.

Beagley, B. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 1999 (*synth, ir, uv, magnetism, cryst struct*)

IC-005382

$C_6H_{18}I_3NiP_2$

Triiodobis(trimethylphosphine)nickel(*III*)

[111943-46-5]

$NiI_3(PMe_3)_2$

M 591.5

Distorted trigonal bipyramidal struct. with axial P, attributed to Jahn-Teller effect. One Ni—I bond (253 pm) shorter than other two (255.1 pm). Black plates (toluene). Sol. C_6H_6. Paramagnetic.

Chandler, D.J. *et al, J. Coord. Chem.*, 1987, **16**, 19 (*synth, cryst struct, ir, esr*)

IC-005383

$C_6H_{18}KNSi_2$

Potassium bis(trimethylsilyl)amide

Bis(trimethylsilyl)amine, potassium salt. Potassium bis(trimethylsilyl)amide, 8CI. 1,1,1-Trimethyl-N-(trimethylsilyl)silanamine, potassium salt, 9CI

[40949-94-8]

$KN(SiMe_3)_2$

M 199.4
Synth. by metallation of bis(trimethylsilyl)amine with a suspension of KH in THF. Commercially available as solid or in soln. in toluene (0.5 mol l^{-1}). Sterically hindered base. Fp 158-162°. Moisture-sensitive. Reacts with H_2O forming the amine and aq. KOH.

▷ Flammable, corrosive.

Brown, C.A., *J. Org. Chem.*, 1974, **39**, 3913 (*synth, uses*)
Marshall, J.A. *et al, J. Am. Chem. Soc.*, 1983, **105**, 5679 (*uses*)

IC-005384

$C_6H_{18}LiNSi_2$

Lithium bis(trimethylsilyl)amide

Bis(trimethylsilyl)amine, lithium salt. Lithium hexamethyldisilazide. 1,1,1-Trimethyl-N-(trimethylsilyl)silanamine lithium salt, 9CI. LTSA

[4039-32-1]

$LiN(SiMe_3)_2$

M 167.3
Mainly dimeric in gas phase. Reagent for metallation of aromatic compds. and/or aryne formn. Base for aldol condensations. Used to generate 2,4-dienolate ions from Δ^4-3-ketosteroids. Sol. THF, hexane. Mp 71-72°. $Bp_{0.01}$ 80-84°.

▷ Flammable.

Dimer: [97587-69-4].
$C_{12}H_{26}Li_2N_2Si_4$ M 324.5
Dimer, bis-Et_2O complex: [84040-90-4]. *Bis[μ-bis(trimethylsilyl)amido(diethyl ether)lithium]*
$C_{20}H_{56}Li_2N_2O_2Si_4$ M 482.8
Tetragonal cryst. (Et_2O). Mp 105-107°.
Dimer, bis-THF complex: [105690-70-8].
$C_{20}H_{52}Li_2N_2O_2Si_4$ M 478.8
White tetragonal cryst. Mp 136-138°.
12-Crown-4 complex (1:1): [92231-06-6].
$C_{14}H_{34}LiNO_4Si_2$ M 343.5
Synth. from 12-crown-4 and hexane soln. of $LiN(SiMe_3)_2$. Triclinic cryst. (THF/Et_2O/hexane).

Inorg. Synth., 1966, **8**, 19 (*synth*)
Mootz, D. *et al, Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 378 (*cryst struct*)
Tanabe, M. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 564 (*uses*)
Neilson, R.H. *et al, Inorg. Chem.*, 1977, **16**, 1455 (*synth*)
Manzer, L.E., *Inorg. Chem.*, 1978, **17**, 1552 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 197 (*use*)
Lappert, M.F. *et al, J. Am. Chem. Soc.*, 1983, **105**, 302 (*struct*)
Engelhardt, L.M. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1671 (*struct*)
Power, P.P. *et al, J. Chem. Soc., Chem. Commun.*, 1984, 358 (*struct*)
Fjeldberg, T. *et al, J. Mol. Struct.*, 1984, **125**, 265 (*ed*)
Engelhardt, L.M. *et al, Aust. J. Chem.*, 1986, **39**, 1337 (*deriv, pmr, cryst struct*)
Fraser, R.R. *et al, Can. J. Chem.*, 1986, **64**, 621 (*use*)
Netka, J. *et al, J. Org. Chem.*, 1986, **51**, 1189 (*use*)
Boeré, R.T. *et al, J. Organomet. Chem.*, 1987, **331**, 161 (*props*)
Renaud, P. *et al, J. Am. Chem. Soc.*, 1988, **110**, 5702 (*props, electrochem*)
Magedov, I.V. *et al, J. Gen. Chem. USSR (Engl. Transl.)*, 1988, **58**, 1727 (*synth*)
Podraza, K.F. *et al, J. Org. Chem.*, 1988, **53**, 2643 (*synth, cmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2150D.

IC-005385

$C_6H_{18}LuN_3O_{12}S_3$

Tris(dimethyl sulfoxide)tris(nitrato)lutetium(*III*)

Tris(nitrato-O,O′)tris[sulfinyl bis[methane]-O]lutetium(III). Tris(dimethyl sulfoxide)lutetium nitrate. Lutetium(III) nitrate tris(dimethyl sulfoxide)

[52518-92-0]

$Lu(NO_3)_3(O{=}SMe_2)_3$

M 595.3
9-Coordinate, with all nitrates bidentate. White cryst. Sol. MeCN, Me_2CO, MeOH, DMSO.

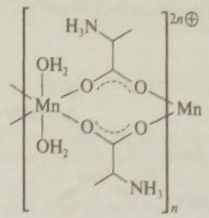
[63903-86-4]

Ramalingam, S.K. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth, ir*)
Aslanov, L.A. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1973, **14**, 998 (*cryst struct*)
Kawano, Y. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 701 (*ir, raman*)
James, B.R. *et al, Spectrochim. Acta, Part A*, 1978, **34**, 577 (*ir*)
Su, Q. *et al, Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581.
Bao, F. *et al, Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

IC-005386

$C_6H_{18}MnN_2O_6^{2\oplus}$

Bis(D,L-α-alanine)diaquamanganese(*II*)(2+)



M 269.1 (ion)
Polymeric cation containing octahedral Mn.

Dibromide:
$C_6H_{18}Br_2MnN_2O_6$ M 428.9
Cryst. + $2H_2O$.

Ciunik, Z. *et al, Inorg. Chim. Acta*, 1980, **44**, L249 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 268 (*rec, bibl*)

IC-005387

$C_6H_{18}MnN_6O_{12}^{2\oplus}$

Hexakis(nitromethane-*O*)manganese(*II*)(2+), 9CI

$[Mn(O_2NMe)_6]^{2\oplus}$

M 421.1 (ion)
Octahedral complex.

Bis-hexachloroantimonate: [26692-38-6]. *Manganese(II) hexachloroantimonate hexakis(nitromethane)*
Synth. from hydrated $MnCl_2$ and $SbCl_5.MeNO_2$ in $MeNO_2$ at r.t. Moisture sensitive white cryst. ($MeNO_2$). Mp 115° (103-107°) dec.

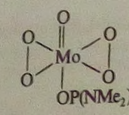
Driessen, W.L. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1969, **88**, 491 (*synth, ir*)
Drăgulescu, C. *et al*, *Monatsh. Chem.*, 1974, **105**, 1176 (*ir, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 21 (*rev, bibl*)

$C_6H_{18}MoO_6P$ IC-005388

(Hexamethylphosphoric triamide-*O*) oxodiperoxymolybdenum

Diperoxooxohexamethylphosphoramidomolybdenum

[25377-12-2]



M 313.1

Reagent for efficient stereospecific epoxidn. of olefins, also for enolate hydroxylation and for oxidn. of alkyl bromides and nitriles. Yellow-orange needles. Mp 101-102° dec. See (Hexamethylphosphoric triamide-*O*) oxodiperoxy(pyridine)molybdenum(*VI*), IC-007340 and Aqua(hexamethylphosphoric triamide-*O*) oxodiperoxymolybdenum, IC-005450.

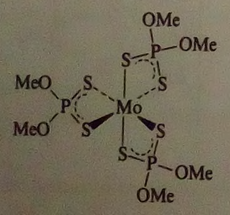
Himoun, H. *et al*, *Tetrahedron*, 1970, **26**, 37 (*synth*)
Sharpless, K.B. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 295 (*use*)
Schmitt, G. *et al*, *J. Organomet. Chem.*, 1978, **152**, 271 (*use*)
Vedjs, E. *et al*, *J. Org. Chem.*, 1978, **43**, 188 (*use*)
Matlin, S.A. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1979, 2481 (*synth, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 206 (*use*)

$C_6H_{18}MoO_6P_3S_6$ IC-005389

Tris(*O,O'*-dimethyldithiophosphato)molybdenum(*III*)

Tris(O,O'-*dimethylphosphorodithioato*-S,S')*molybdenum*(III), *11CI*

[85214-72-8]



M 567.4

Rare monomeric Mo(*III*) complex with S ligation only. Mo(*III*) precursors usually react with thiols to give thiolato- or sulfido-bridged oligomers. Red needles (CH_2Cl_2/Et_2O).

Dilworth, J.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 397 (*cryst struct, synth*)

$C_6H_{18}NNaSi_2$ IC-005390

Sodium bis(trimethylsilyl)amide

*1,1,1-Trimethyl-*N*-(trimethylsilyl)silanamine, sodium salt, 8CI. N-Sodiohexamethyldisilazane. Sodium hexamethyldisilazide. Sodium hexamethyldisilylamide*

[1070-89-9]

$$NaN(SiMe_3)_2$$

M 183.3

Synth. from $(Me_3Si)_2NH$ + NaH. Commercially available. Useful non-nucleophilic base; electron transfer reagent. Moisture-sensitive white monoclinic cryst., powder. Sol. THF, hydrocarbons. Mp 171-175°. Bp_2 170°.

▷ Corrosive.

Et_2O complex:

$C_{10}H_{28}NNaOSi_2$ M 257.4
Mp 72-74°.

THF complex:

$C_{10}H_{26}NNaOSi_2$ M 255.4
Mp 70-85° dec.

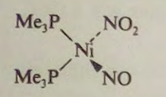
Fessenden, R.W., *J. Org. Chem.*, 1960, **25**, 2191 (*ir*)
Wannagat, U. *et al*, *Chem. Ber.*, 1961, **94**, 1540 (*synth, props, derivs*)
Kruger, C. *et al*, *Chem. Ber.*, 1963, **96**, 2132 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1046; **3**, 261; **4**, 442; **6**, 529; **7**, 329; **12**, 441 (*use*)
Wannagat, U., *Pure Appl. Chem.*, 1969, **19**, 329 (*rev, synth*)
Moll, M. *et al*, *Z. Naturforsch., B*, 1976, **31**, 1019 (*uses*)
Gruening, R. *et al*, *J. Organomet. Chem.*, 1977, **137**, 101 (*cryst struct*)
Evans, D.A. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 6757 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3130D (*haz*)
Stork, G. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2173 (*use*)
Gaudemar, M. *et al*, *Tetrahedron Lett.*, 1989, **30**, 2779 (*use*)

$C_6H_{18}N_2NiO_3P_2$ IC-005391

(Nitrito-*N*)nitrosylbis(trimethylphosphine)nickel(*II*), 11CI

Nitrosyl(*nitro*)*bis*(*trimethylphosphine*)*nickel*(II)

[79499-32-4]



M 286.8

Distorted tetrahedral struct. which is in equilibrium in soln. with *O*-bonded $NO_2^{\ominus}$. Synth. from $Ni(NO_2)_2(PMe_3)_2$ + CO in Me_2CO. Blue-black cryst. (Et_2O). Sol. $CHCl_3$.

Kriege-Simondsen, J. *et al*, *Inorg. Chem.*, 1982, **21**, 230; 1983, **22**, 3318 (*synth, ir, uv, P-31 nmr, cryst struct*)

$C_6H_{18}N_3OP$ IC-005392

Hexamethylphosphoric triamide, 9CI

Hexamethylphosphoramide. Tris(dimethylamido) oxophosphorus(V). *HMPT*

[680-31-9]

$$OP(NMe_2)_3$$

M 179.2

Widely used as polar, aprotic solvent which activates the synth. and use of organometallic compds. (e.g. Li, Mg derivs.). Widespread use in organic synthesis: converts benzamides into dimethylaminoquinolines, dehydrating agent for alcohols and amides. Used in combination with $SOCl_2$ for synth. of alkyl chlorides. Used for extraction separation of metals ($CHCl_3$, as SCN-complexes); photometric detn. of Os, Ru, Fe(*III*), Ti. Liq. Misc. H_2O. d_4^{20} 1.025. Mp 7°. Bp 235°, Bp_{15} 115°, Bp_1 68-70°. n_D^{20} 1.4582.

▷ Potent animal carcinogen; suspected human carcinogen. Irritant. TD0875000.

Normant, H., *Angew. Chem., Int. Ed. Engl.*, 1967, **6**, 1046 (*rev*)
Diggle, J.W. *et al*, *J. Phys. Chem.*, 1974, **78**, 1018 (*props*)

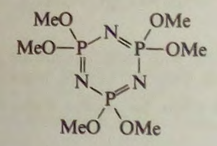
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 323; 1977, **6**, 273; 1979, **7**, 168; 1980, **8**, 240; 1981, **9**, 235; 1982, **10**, 196.
Gloe, K. *et al*, *J. Prakt. Chem.*, 1975, **317**, 529 (*synth*)
Pantzer, R. *et al*, *Z. Anorg. Allg. Chem.*, 1975, **416**, 297 (*ir, raman*)
Mitra, M. *et al*, *Anal. Chim. Acta*, 1977, **94**, 489 (*Ti*)
London, A.G. *et al*, *Org. Mass Spectrom.*, 1977, **12**, 283 (*ms*)
Mitra, M. *et al*, *Talanta*, 1977, **24**, 698; 1978, **25**, 599 (*use*)
Pederson, E.B., *CA*, 1978, **89**, 89752e (*rev*)
Itaya, K. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 5996 (*purifn*)
Spencer, H., *Chem. Ind. (London)*, 1979, 728 (*tox*)
Chowdhury, R.P. *et al*, *Mikrochim. Acta*, 1979, **2**, 515 (*detn, Fe*)
Bergesen, K. *et al*, *Acta Chem. Scand., Ser. A*, 1981, **35**, 147 (*cmr*)
Pal, B.K. *et al*, *Talanta*, 1981, **28**, 62 (*detn, Os*)
Cowley, A.H. *et al*, *Inorg. Chem.*, 1982, **21**, 543 (*pe*)
Worley, S.D. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1982, **25**, 135 (*pe, struct*)
Mitra, B.K. *et al*, *Mikrochim. Acta*, 1982, **2**, 449 (*detn, Ru*)
Duangthai, S. *et al*, *Org. Magn. Reson.*, 1982, **20**, 33 (*struct*)
Fujinaga, T. *et al*, *Recomm. Methods Purif. Solvents Tests Impurities*, (J.F. Coetzee Ed.), Pergamon, 1982, 38 (*rev*)
Koidan, G.N. *et al*, *Zh. Obshch. Khim.*, 1982, **52**, 2001; *J. Gen. Chem. USSR (Engl. Transl.)*, 1982, **52**, 1779 (*synth, props, derivs*)
Cload, P.A. *et al*, *Org. Mass Spectrom.*, 1983, **18**, 57 (*ms*)
Bollinger, J.-C. *et al*, *Org. Mass Spectrom.*, 1985, **20**, 318 (*ms*)
Appling, J.R. *et al*, *Org. Mass Spectrom.*, 1985, **20**, 343 (*ms*)
Bollinger, J.-C. *et al*, *Spectrochim. Acta, Part A*, 1985, **41**, 399 (*pmr, ir*)
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 346.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1870.

$C_6H_{18}N_3O_6P_3$ IC-005393

2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexamethoxy-1,3,5,2,4,6-triazatriphosphorine, 9CI, 8CI

2,2,4,4,6,6-Hexamethoxy-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine. 2,2,4,4,6,6-Hexamethoxy-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene

[957-13-1]



M 321.1

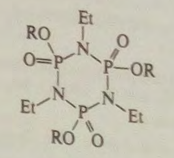
Synth. from 2,2,4,4,6,6-Hexachloro-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, IC-017314 + NaOMe. White cryst. (Et_2O/pet. ether). Mp 48° (45-46°).

Fitzsimmons, B.W. *et al*, *J. Chem. Soc.*, 1964, 1735 (*synth*)
Feakins, D. *et al*, *J. Chem. Soc.*, 1965, 2804 (*props*)
Branton, G.R. *et al*, *J. Chem. Soc. A*, 1970, 151 (*pe*)
Kajiwara, M. *et al*, *Polymer*, 1976, **17**, 898 (*uv, P-31 nmr*)
Mason, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2337 (*N-14 nmr, P-31 nmr*)
Cheng, T.C. *et al*, *Macromolecules*, 1980, **13**, 158 (*reactions, cmr, P-31 nmr*)
Ferrar, W.T. *et al*, *Macromolecules*, 1980, **13**, 1345 (*synth*)
Dhathathreyan, K.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1928 (*pmr, cmr, P-31 nmr*)
Thomas, B. *et al*, *Phosphorus Sulfur*, 1981, **10**, 375 (*N-15 nmr, P-31 nmr*)

$C_6H_{18}N_3O_6P_3$ IC-005394

1,3,5-Triethyl-1,2,3,4,5,6-hexahydro-2,4,6-trihydroxy-1,3,5,2,4,6-triazatriphosphorine 2,4,6-trioxide

1,3,5-Triethyl-2,4,6-trihydroxycyclotriazaphosphane 2,4,6-trioxide



R = H

M 321.1

O,O',O''-*Triethyl*: [84227-56-5]. *2,4,6-Triethoxy-1,3,5-triethyl-1,2,3,4,5,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine 2,4,6-trioxide*
$C_{12}H_{30}N_3O_6P_3$ M 405.3
Colourless cryst. (pet. ether). Mp 74-75°.

O,O',O''-*Triisopropyl*: *1,3,5-Triethyl-1,2,3,4,5,6-hexahydro-2,4,6-triisopropoxy-1,3,5,2,4,6-triazatriphosphorine 2,4,6-trioxide*
$C_{15}H_{36}N_3O_6P_3$ M 447.3
Colourless cryst. (pet. ether). Mp 150-152°.

O,O'O''-*Tris*(*4-nitrobenzyl*):
$C_{27}H_{33}N_6O_{12}P_3$ M 726.5
Pale yellow cryst. (EtOH). Mp 168-169°.

Fitzsimmons, B.W. *et al*, *J. Chem. Soc.*, 1965, 7432 (*synth, ir*)
Thomas, B. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **490**, 121 (*ir, N-15 nmr, P-31 nmr*)

$C_6H_{18}N_3O_{12}S_3Tb$ IC-005395

Tris(dimethyl sulfoxide)tris(nitrato)terbium(*III*)

Tris(*nitrato*-O,O')*tris*[*sulfinylbis*[*methane*]-O]*terbium*(III), *9CI. Terbium*(III) *nitrate tris*(*dimethyl sulfoxide*)

[57425-83-9]

$$Tb(NO_3)_3(O{=}SMe_2)_3$$

M 579.3

Assumed to be 9-coordinate. Isomorphous with Yb analogue. Colourless cryst. Sol. MeCN, Me_2CO, MeOH, DMSO.

Bhandary, K.K. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 1997 (*struct*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581 (*synth*)
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

$C_6H_{18}N_3O_{12}S_3Tm$ IC-005396

Tris(dimethyl sulfoxide)tris(nitrato)thulium(*III*)

Tris(*nitrato*-O,O')*tris*[*sulfinylbis*[*methane*]-O]*thulium*(III), *11CI, 9CI. Thulium*(III) *nitrate tris*(*dimethyl sulfoxide*)

[57425-84-0]

$$Tm(NO_3)_3(O{=}SMe_2)_3$$

M 589.3

Presumed 9-coordinate, isomorphous with Yb analogue. Green cryst. Sol. MeCN, Me_2CO, MeOH, DMSO.

Bhandary, K.K. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 1997 (*struct*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581 (*synth*)
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

$C_6H_{18}N_3O_{12}S_3Y$ IC-005397

Tris(dimethyl sulfoxide)tris(nitrato)yttrium(*III*)

Tris(nitrato-O,O′)tris[sulfinylbis[methane]-O]yttrium(III), *11Cl. Yttrium*(III) *nitrate tris(dimethyl sulfoxide)*

[86593-24-0]

$Y(NO_3)_3(O{=}SMe_2)_3$

M 509.3

9-Coordinate, all nitrates bidentate. White cryst. Sol. MeCN, Me_2CO, MeOH, DMSO. Mp 155°.

[13963-72-9, 19633-60-4]

Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth, ir*)

Lin, Y. *et al*, *Wuli Xuebao*, 1983, **32**, 400; *CA*, **99**, 62065 (*cryst struct*)

Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, 1985, **103**, 31581 (*synth*)

Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

$C_6H_{18}N_3O_{12}S_3Yb$ IC-005398

Tris(dimethyl sulfoxide)tris(nitrato)ytterbium(*III*)

Tris(nitrato-O,O′)tris[sulfinylbis[methane]-O]ytterbium(III). *Tris(dimethyl sulfoxide)ytterbium nitrate. Ytterbium*(III) *nitrate tris(dimethyl sulfoxide)*

[55450-35-6]

$Yb(NO_3)_3(O{=}SMe_2)_3$

M 593.4

9-Coordinate with all nitrates bidentate. Yellow cryst. Sol. MeCN, Me_2CO, MeOH, DMSO. Mp 163°.

[18460-09-8, 39914-76-6]

Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth, ir*)

Bhandary, K.K. *et al*, *Cryst. Struct. Commun.*, 1973, **2**, 99 (*cryst struct*)

Bhandary, K.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 288.

Kawano, Y. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 701 (*ir, raman*)

James, B.R. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 577 (*ir*)

Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

$C_6H_{18}N_3Sb$ IC-005399

Tris(dimethylamino)stibine, 8CI

Hexamethylstibinetriamine, 9CI. Tris(dimethylamido) antimony

[7289-92-1]

$Sb(NMe_2)_3$

M 253.9

Liq. $Bp_{0.45}$ 32-34°.

Moedritzer, K., *Inorg. Chem.*, 1964, **3**, 609 (*synth, pmr*)

George, T.A. *et al*, *J. Chem. Soc. A*, 1969, 992 (*synth*)

Kiennemann, A. *et al*, *J. Organomet. Chem.*, 1972, **35**, 143 (*synth, ir, props*)

Kiennemann, A. *et al*, *Bull. Soc. Chim. Fr.*, 1975, 1185 (*props*)

Ensinger, U. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **514**, 137; 1985, **520**, 160 (*ir, raman, ms*)

Ando, F. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 1564 (*reactions*)

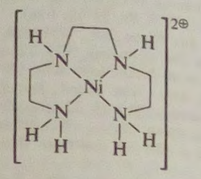
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 3422.

$C_6H_{18}N_4Ni^{2\oplus}$ IC-005400

(Triethylenetetramine)nickel(*II*)(2+), 8CI

1,4,7,10-Tetraazadecanenickel(II)(2+). [N,N′-*Bis*(2-*aminoethyl*)-*1,2-ethanediamine*]*nickel*(II)(2+), *9CI. (Trien)nickel*(2+). *(2,2,2-Tet)nickel*(2+)

[24653-01-8]



M 204.9 (ion)

Square planar struct. Forms octahedral complexes with coordinating anions e.g. Bis(thiocyanato-*N*)(triethylenetetramine)nickel(*II*), IC-006154; also forms dinuclear Ni(*II*) complexes e.g. Tris(triethylenetetramine)dinickel(*II*)(4+), IC-010228. Orange solns. in non-donor solvs., blue solns. in donor solvs., indicating octahedral coordn.

Diperchlorate: [15609-09-3].
$C_6H_{18}Cl_2N_4NiO_8$ M 403.8
Hygroscopic orange cryst.
▷ Potentially explosive.

Curtis, N.F. *et al*, *J. Chem. Soc.*, 1965, 619 (*synth, ir*)

McPherson, A. *et al*, *J. Coord. Chem.*, 1971, **1**, 39 (*cryst struct*)

$C_6H_{18}N_4NpO_{15}S_3$ IC-005401

Tris(dimethyl sulfoxide)tetrakis(nitrato)neptunium(*IV*)

Tetrakis(nitrato-O,O′)tris[sulfinylbis[methane]-O] neptunium(IV). *Neptunium*(IV) *chloride tris(dimethyl sulfoxide)*

[52394-53-3]

$Np(NO_3)_4(O{=}SMe_2)_3$

M 719.4

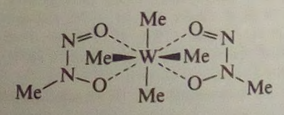
Probably 11-coord. with bidentate nitrate groups. Grey-green solid. Sol. Me_2CO, MeCN, $MeNO_2$.

Alvey, J.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2326 (*synth, ir*)

$C_6H_{18}N_4O_4W$ IC-005402

Tetramethylbis(*N*-methyl-*N*-nitrosohydroxylaminato) tungsten(*VI*), 9CI

[40846-52-4]



M 394.0

Example of an 8-coordinate W(*VI*) compd. Geometry intermed. between dodecahedral and square antiprismatic. Synth. from WMe_6 + NO. Air-sensitive yellow prisms (toluene).

Fletcher, S.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1972, 922 (*cryst struct, pmr, synth*)

$C_6H_{18}N_4O_{15}PuS_3$ IC-005403

Tris(dimethyl sulfoxide)tetrakis(nitrato)plutonium(*IV*)

Tetranitratotris[sulfinylbis[methane]-O]plutonium(IV). *Plutonium*(IV) *nitrate tris(dimethyl sulfoxide)*

[52394-54-4]

$Pu(NO_3)_4(O{=}SMe_2)_3$

M 721.4

Presumed 11-coordinate with bidentate nitrates. Green solid.

Alvey, J.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2326 (*synth, ir, uv*)

$C_6H_{18}N_4O_{15}S_3Th$ IC-005404

Tris(dimethyl sulfoxide)tetrakis(nitrato)thorium(*IV*)

Tetrakis(nitrato-O,O′)tris[sulfinylbis[methane]-O] thorium(IV). *Thorium*(IV) *nitrate tris(dimethyl sulfoxide)*

[52479-32-0]

$Th(NO_3)_4(O{=}SMe_2)_3$

M 714.4

11-Coord. capped pentagonal prismatic geometry with bidentate nitrate ligands. White cryst. (Me_2CO/2-methylbutane or Me_2CO). Sol. Me_2CO, MeCN, $MeNO_2$. Obt. as three cryst. mods. depending on solv.

[37322-48-8]

Alvey, J.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2326 (*synth, ir, cryst struct*)

$C_6H_{18}N_4O_{15}S_3U$ IC-005405

Tris(dimethyl sulfoxide)tetrakis(nitrato)uranium(*IV*)

Tetrakis(nitrato-O,O′)tris[sulfinylbis[methane]-O] uranium(IV). *Uranium*(IV) *nitrate tris(dimethyl sulfoxide)*

[52394-55-5]

$U(NO_3)_4(O{=}SMe_2)_3$

M 720.4

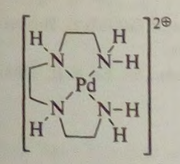
Probably 11-coord. with bidentate nitrates. Pale green solid. Sol. Me_2CO. Oxidises rapidly in soln.; in solid state, within a few hrs. on standing.

Alvey, J.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2326 (*synth, ir*)

$C_6H_{18}N_4Pd^{2\oplus}$ IC-005406

(Triethylenetetramine)palladium(*II*)(2+)

[N,N′-*Bis*(2-*aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴] *palladium*(2+), *9CI*



M 252.6 (ion)

Diperchlorate: [62157-30-6].
Yellow needles (H_2O).
▷ Potentially explosive.

Bis-hexafluorophosphate: [62157-29-3].
Yellow needles + $1KPF_6$ (aq. EtOH).

Tetrachloropalladate(2−):
$C_6H_{18}Cl_4N_4Pd_2$ M 500.8
Light-tan powder. Mp 230-235° dec.

Jonassen, H.B. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 4097 (*synth*)

Hori, F. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 138 (*synth, cryst struct, uv*)

$C_6H_{18}N_5O_{17}P_2Th^{\ominus}$ IC-005407

Pentanitratobis(trimethylphosphine oxide)thorate(*IV*)

Pentakis(nitrato-O,O′)bis(trimethylphosphine oxide-O) thorate(IV)(1−), *10Cl*

$[Th(NO_3)_5(O{=}PMe_3)_2]^{\ominus}$

M 726.2 (ion)

12-Coordinate anion.

Ph_4P salt: [67840-61-3].
Colourless cryst. (Me_2CO/EtOH). Sol. Me_2CO. Mp 180°.

Alcock, N.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 638 (*synth, ir, cryst struct*)

$C_6H_{18}N_6NiO_{12}^{2\ominus}$ IC-005408

Hexakis(nitromethane)nickel(*II*)(2+), 8CI

$[Ni(MeNO_2)_6]^{2\ominus}$

M 424.9 (ion)

Octahedral struct. Starting material for synth. of other $[NiL_6]^{2\ominus}$ complexes (L = O donor).

Bis-hexachloroantimonate salt: [26539-76-4].
$C_6H_{18}Cl_{12}N_8NiO_{12}Sb_2$ M 1093.8
Green solid.

Driersen, W.L. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1969, **88**, 491 (*synth, ir, uv*)

$C_6H_{18}N_6P^{\ominus}$ IC-005409

Azidotris(dimethylamino)phosphorus(1+)

Azidotris(N-*methylmethanaminato*)*phosphorus*(1+), *9Cl*

$(Me_2N)_3PN_3^{\ominus}$

M 205.2 (ion)

Reagent for coupling of peptides, converts carboxylic acids into acyl azides.

Hexafluorophosphate: [50281-51-1].
Cryst. (Me_2CO/Et_2O). Mp >250°.

Chloride: [124167-48-2].
Cryst. (THF/CH_2Cl_2). Mp 162° dec.

Castro, B. *et al*, *Bull. Soc. Chim. Fr.*, Part 2, 1973, 3359 (*synth, ir, pmr, use*)

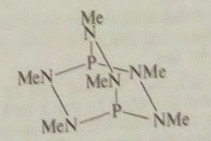
Castro, B. *et al*, *Tetrahedron Lett.*, 1973, 3243 (*synth*)

Marchenko, A.P. *et al*, *Zh. Obshch. Khim.*, 1988, **58**, 2230; *J. Gen. Chem. USSR* (*Engl. Transl.*), 1988, **58**, 1985 (*synth*)

$C_6H_{18}N_6P_2$ IC-005410

2,3,5,6,7,8-Hexamethyl-2,3,5,6,7,8-hexaaza-1,4-diphosphabicyclo[2.2.2]octane, 9CI, 8CI

[3478-74-8]



M 236.1

Solid. Mp 120-121°. $Subl._{0.001}$ 70°.

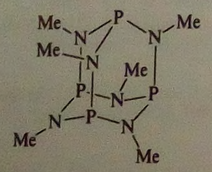
1,4-Dioxide: [3182-66-9].
$C_6H_{18}N_6O_2P_2$ M 268.1
Cryst. (toluene). Mp 316° (320-325°).

1,4-Disulfide: [3335-14-6].
$C_6H_{18}N_6P_2S_2$ M 300.3
Cryst. (toluene). Mp 340°. Sinters at 270°.
1,4-Diselenide: [38167-29-2].
$C_6H_{18}N_6P_2Se_2$ M 394.1
Solid. Mp 340°.

van Doone, W. *et al, Inorg. Chem.*, 1971, **10**, 2591 (*cryst struct*)
Goetze, R. *et al, Chem. Ber.*, 1972, **105**, 2637 (*synth, derivs, ms, ir, pmr, P-31 nmr*)
Havlicek, M.D. *et al, Inorg. Chem.*, 1972, **11**, 1624 (*synth, ir, pmr, props*)
Gilje, J.W. *et al, Inorg. Chem.*, 1972, **11**, 1643 (*dioxide, cryst struct*)
Nöth, H. *et al, Chem. Ber.*, 1974, **107**, 1019; 1976, **109**, 1942 (*synth, pmr, N-15 nmr, P-31 nmr*)
Cowley, A.H. *et al, Inorg. Chem.*, 1977, **16**, 854 (*pe*)
Bulloch, G. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 764 (*pmr, cmr*)

$C_6H_{18}N_6P_4$ IC-005411

2,4,6,8,9,10-Hexamethyl-2,4,6,8,9,10-hexaaza-1,3,5,7-tetraphosphatricyclo[3.3.1.1^{3,7}]decane, 10CI, 9CI
closo-*Tetraphosphorus hexakis(methylimide). 2,4,6,8,9,10-Hexamethyl-2,4,6,8,9,10-hexaaza-1,3,5,7-tetraphosphaadamantane*
[10369-17-2]

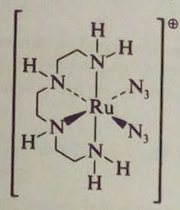


M 298.1
Solid. Mp 122-123°. Bp_{737} 303-304°.
1,3,5,7-Tetroxide: [58979-11-6].
$C_6H_{18}N_6O_4P_4$ M 362.1
Solid. Mp 179° dec. $Subl._{0.001}$ 180°.
1-Sulfide: [38448-57-6].
$C_6H_{18}N_6P_4S$ M 330.2
Cryst. (pentane). Mp 94°. Polymorphous.
1,3-Disulfide: [38448-56-5].
$C_6H_{18}N_6P_4S_2$ M 362.2
Cryst. (pentane). Mp 125-126°.
1,3,5-Trisulfide: [38448-55-4].
$C_6H_{18}N_6P_4S_3$ M 394.3
Cryst. (pentane). Mp 174°.
1,3,5,7-Tetrasulfide: [37747-07-2].
$C_6H_{18}N_6P_4S_4$ M 426.4
Cryst. ($CHCl_3$/pentane). Mp 246°.
1-Oxide, 3,5,7-Trisulfide:
$C_6H_{18}N_6OP_4S_3$ M 410.3
Solid. Mp 215° dec.
1,3-Dioxide, 5,7-Disulfide:
$C_6H_{18}N_6O_2P_4S_2$ M 394.2
Solid. Mp 185° dec.
1,3,5-Trioxide, 7-Sulfide:
$C_6H_{18}N_6O_3P_4S$ M 378.2
Solid. Mp 157° dec.

Holmes, R.R. *et al, J. Am. Chem. Soc.*, 1961, **83**, 1334 (*synth*)
Wolff, A. *et al, Bull. Soc. Chim. Fr.*, Part I, 1973, 1587.
Elkain, J.C. *et al, Phosphorus*, 1973, **2**, 249 (*derivs, P-31 nmr*)
Wolff, A. *et al, Org. Mass Spectrom.*, 1974, **9**, 594 (*ms*)
Riess, J.G. *et al, Inorg. Chim. Acta*, 1976, **17**, L27 (*tetraoxide, pmr, P-31 nmr*)
Casabianca, F. *et al, Inorg. Chem.*, 1977, **16**, 864 (*derivs, synth, ir, ms, pmr*)
Casabianca, F. *et al, Inorg. Chem.*, 1978, **17**, 3232 (*tetraoxide, tetrasulfide, cryst structs*)
Cotton, F.A. *et al, Inorg. Chem.*, 1978, **17**, 3521 (*monosulfide, cryst struct*)
Bulloch, G. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 764 (*pmr, cmr*)
Lee, T.H. *et al, J. Am. Chem. Soc.*, 1980, **102**, 2631 (*pe*)
Cotton, F.A. *et al, Inorg. Chem.*, 1982, **21**, 3123 (*sulfides, cryst struct*)
Cotton, F.A. *et al, Inorg. Chem.*, 1983, **22**, 133 (*pe, cmr*)

$C_6H_{18}N_{10}Ru^{\oplus}$ IC-005412

Diazido(triethylenetetramine)ruthenium(*III*)(1+), 8CI
Bis(azido)(1,8-diamino-3,6-diazaoctane)ruthenium(III)(*1+*)



M 331.3 (ion)
Dec. both in soln. and in the solid state (as salt) with evolution of N_2, prob. via a nitrene intermed.
Hexafluorophosphate: [30468-61-2].
Prepd. by metathesis of corresp. dichloro Ru deriv. using $Ag^{\oplus}$, followed by $N_3^{\ominus}$ and $[PF_6]^{\ominus}$. May be stored at −15° in the dark for several weeks. Purple-red cryst. μ_{eff} = 1.9 μ_B. Ir μ_{N_3} 2050, 2030 cm^{-1}.

Kane-Maguire, L.A.P. *et al, J. Am. Chem. Soc.*, 1970, **92**, 5865 (*synth, ir, uv, magnetism*)

$C_6H_{18}O_2PbSi_2$ IC-005413

Bis(trimethylsilyloxy)lead

$Pb(OSiMe_3)_2$

M 385.5
Shiny cryst. (THF). Sol. THF, CH_2Cl_2, pentane, C_6H_6, toluene. Mp 160°.

Du Mont, W.W. *et al, Chem. Ber.*, 1981, **114**, 1180.

$C_6H_{18}O_6Re$ IC-005414

Hexamethoxyrhenium(*VI*)
Hexamethoxorhenium(VI). *Rhenium*(VI) *methoxide*

$Re(OMe)_6$

M 372.4
Synth. from ReF_6 and $Si(OMe)_4$. Brown solid. Mp 59°. Subl. 30° *in vacuo*.

Jacob, E., *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 242 (*synth, ir, props*)

$C_6H_{18}O_6Tc^{2\ominus}$ IC-005415

Hexamethoxytechnetate(*IV*)(2−)

$[Tc(OMe)_6]^{2\ominus}$ (O_h)

M 285.1 (ion)
Synth. by reaction of $TcBr_6^{2\ominus}$ with $OMe^{\ominus}$ in MeOH. Dec. in aq. soln. if pH < 12; oxidises in air.
Di-K salt: [107827-93-0].
White solid. Sol. MeOH, EtOH; insol. other org. solvs.

Alberto, R. *et al, Polyhedron*, 1986, **5**, 2107 (*synth, ir, uv, props*)

$C_6H_{18}O_6U$ IC-005416

Hexamethoxyuranium(*VI*)
Uranium(VI) *methoxide. Uranium hexamethoxide*
[69644-82-2]

$U(OMe)_6$

M 424.2
Molecular. Used as intermed. in laser induced separation of ^{235}U and ^{238}U, ten times more efficient than gaseous diffusion. V. moisture-sensitive dark-red cryst.; sl. light-sensitive. Sol. C_6H_6, CH_2Cl_2, pentane, CCl_4. Mp 70-72° (62-64°). $Subl._{0.00001}$ 30°. A range of fluoroderivs $UF_n(OMe)_{6-n}$ also can be obt. V.p. 3.8 × 10^{-3} mm (25°).
[83178-44-3]

Jacob, E., *Z. Anorg. Allg. Chem.*, 1977, **433**, 255 (*use*)
U.S. Pat., 4097384, (1978); *CA*, **89**, 170739 (*use*)
Miller, S.S. *et al, J. Am. Chem. Soc.*, 1979, **101**, 1036 (*synth, ir, raman, pmr*)
Paine, R.T. *et al, ACS Symp. Ser.*, 1980, **131**, 369 (*use*)
Cuellar, F.A. *et al, Inorg. Chem.*, 1981, **20**, 2129 (*synth, uv-vis, ms*)
Jacob, E., *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 142 (*synth, ir, raman, ms, pmr*)
Cuellar, E.A. *et al, J. Am. Chem. Soc.*, 1983, **105**, 4580 (*synth, ir, raman, cryst struct*)

$C_6H_{18}O_6W$ IC-005417

Hexamethoxytungsten(*VI*)
Hexamethoxotungsten(VI). *Tungsten*(VI) *methoxide*
[35869-33-1]

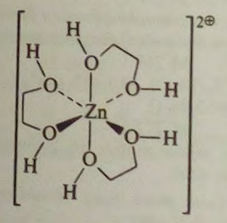
$W(OMe)_6$ (O_h)

M 370.0
Several homologues known. Synth. from Hexakis(dimethylamido)tungsten(*VI*), IC-008287 and MeOH in hexane; or from $W(NMe_2)_3(OMe)_3$ in C_6H_6. White cryst. (pentane). Sol. C_6H_6. $Subl._{0.001}$ 50-60°.

Bradley, D.C. *et al, Inorg. Chem.*, 1977, **16**, 1794 (*synth, ir, raman, pmr, cmr, ms*)

$C_6H_{18}O_6Zn^{2\oplus}$ IC-005418

Tris(1,2-ethanediol-*O,O'*)zinc(*II*)(2+)
Tris(ethyleneglycol)zinc(II)(*2+*)

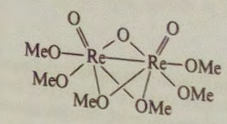


M 251.5 (ion)
Octahedral cation.
Sulfate: [59245-97-5]. *Zinc*(II) *sulfate tris(ethyleneglycol)*
Hygroscopic cryst.

Antti, B.-M., *Acta Chem. Scand., Ser. A*, 1976, **30**, 103 (*synth, cryst struct*)

$C_6H_{18}O_9Re_2$ IC-005419

Hexamethoxytrioxodirhenium(*VI*)
Di-μ-methoxytetramethoxy-μ-oxodioxodirhenium(VI), *10CI*
[73330-12-8]

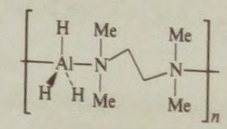


M 606.6
Re=O 169, 170.3, Re—Re 255.9 pm. Synth. from $ReOCl_4$ in MeOH in presence of a *tert*-amine. Orange, air-sensitive cryst. Diamagnetic with Re—Re single bond.

Edwards, P.G. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 2467 (*synth, ir, magnetism, cryst struct*)

$C_6H_{19}AlN_2$ IC-005420

Aluminium hydride tetramethylethylenediamine
N,N,N′,N′-*Tetramethylethylenediamine-alane. Trihydro*(N,N,N′,N′-*tetramethylethylenediamine*)*aluminium, 8CI*
[32995-50-9]



M 146.2
Several similar compds. descr. White air- and moisture-sensitive needles (by subl.). V.p. 1.5 mm at 99°. ΔH_f° −108 kJ mol^{-1}.

Davidson, J.M. *et al, J. Am. Chem. Soc.*, 1960, **82**, 5506 (*synth*)
Palenik, G.J., *Acta Crystallogr.*, 1964, **17**, 1573 (*cryst struct*)
Greenwood, N.N. *et al, J. Chem. Soc. A*, 1971, 814 (*thermodyn*)

$C_6H_{19}BN_2$ IC-005421

Trihydro(*N,N,N′,N′*-tetramethyl-1,2-ethanediamine-*N*)boron, 10CI
Borane tetramethylethylenediamine. N,N,N′,N′-*Tetramethylethylenediamine compd. with borane(1:1). TMED* BH_3
[5843-32-3]

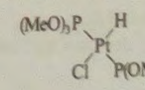
$Me_2NCH_2CH_2NMe_2{-}BH_3$

M 130.0
White cryst. solid. Can be stored below m.p. at least 24 hrs. Above m.p. quickly dec. in absence of excess TMED.

Gatti, A.R. *et al, Inorg. Chem.*, 1966, **5**, 329 (*synth, nmr*)
Brown, H.C. *et al, Inorg. Chem.*, 1980, **19**, 455.

$C_6H_{19}ClO_6P_2Pt$ IC-005422

Chlorohydrobis(trimethyl phosphite-*P*)platinum, 11CI
Bis(trimethylphosphite)chlorohydridoplatinum



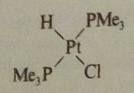
M 479.6

trans-form [90838-78-1]
Cryst. (Et_2O); stable in soln. but solid dec. readily. Ir ν_{Pt-H} 2050 cm^{-1}.

Meyer, W.R. *et al, Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 529 (*synth, ir, pmr, Pt-195 nmr, P-31 nmr*)

$C_6H_{19}ClP_2Pt$ IC-005423

Chlorohydrobis(trimethylphosphine)platinum, 11Cl
Bis(trimethylphosphine)platinum hydridochloride.
Hydridochlorobis(trimethylphosphine)platinum



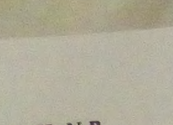
M 383.6

trans-form [91760-38-2]
Olefin isomerisation catalyst. Cryst. (C_6H_6/hexane). Mp 132-137° dec., Mp 164-165° (sealed tube). Ir ν_{Pt-H} 2185 cm^{-1}. Early reports of use as anti-Markownikoff hydration catalyst appear to be incorrect.

Chatt, J. *et al, J. Chem. Soc.*, 1962, 5075 (*synth, ir*)
Flood, T.C. *et al, Organometallics*, 1984, **3**, 1795 (*synth, ir, pmr, P-31 nmr*)
Ramprasad, D. *et al, Inorg. Chem.*, 1988, **27**, 3151 (*synth, pmr, P-31 nmr, props*)

$C_6H_{19}Cl_3N_3Ta$ IC-005424

Trichlorobis(dimethylamido)(dimethylamine)tantalum(*V*)
Trichlorobis(N-*methylmethanaminato*)(N-*methylmethanamine*)*tantalum*(V), *10Cl*
[77071-69-3]

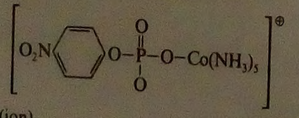


M 420.5
mer-Octahedral. Synth. by adding $HNMe_2$ to $TaCl_5$ in C_6H_6, filtering and adding pentane. Red solid. Sol. C_6H_6.

Chisholm, M.H. *et al, Inorg. Chem.*, 1981, **20**, 1859 (*synth, cryst struct, ir, pmr, ms*)

$C_6H_{19}CoN_6O_6P^{\oplus}$ IC-005425

Pentaammine[mono(4-nitrophenyl)phosphato(2−)-*O*]cobalt(*III*)(1+), 10Cl
p-*Nitrophenylphosphatopentamminecobalt*(III)(*1+*)

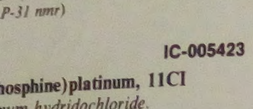


M 361.1 (ion)
Base hydrolysis of this cation has been studied.
Chloride: [75325-33-6].
Red-orange cryst. Sol. H_2O.

Harrowfield, J.M. *et al, J. Am. Chem. Soc.*, 1980, **102**, 7733 (*synth, uv, pmr, cmr*)

$C_6H_{19}CoN_7^{3\oplus}$ IC-005426

Pentaammine(4-cyanopyridine)cobalt(*III*)
Pentaammine(*isonicotinonitrile*)*cobalt*(*3+*), *8Cl*.
Pentaammine(*4-pyridinecarbonitrile*)*cobalt*(*3+*), *9Cl*



Py-bonded form

M 248.1 (ion)
Exhibits linkage isomerism.

Nitrile-bonded-form [53739-10-9]
Triperchlorate: [53739-11-0].
Yellow cryst. (H_2O).
N-*Oxide, triperchlorate:* [120712-09-6]. *Pentaammine(4-pyridinecarbonitrile 1-oxide-*N^4*)cobalt(3+) perchlorate, 9Cl*
Yellow cryst. ($HClO_4$ aq.).

Pyridine-bonded-form [46247-07-8]
Triperchlorate: [25517-40-2].
Large deep-orange cryst.

Balahura, R.J., *Can. J. Chem.*, 1974, **52**, 1762 (*synth, isom, ir, uv, pmr*)
Szecsy, A.P. *et al, J. Am. Chem. Soc.*, 1982, **104**, 3063 (*synth*)
Purcell, W.L., *Inorg. Chem.*, 1989, **28**, 2312 (*synth, N-oxide*)

$C_6H_{19}N_4P$ IC-005427

***N,N,N′,N′,N″,N″*-Hexamethylphosphorimidic triamide, 9Cl**
P,P,P-*Tris*(*dimethylamino*)*phosphine imide*. P,P,P-*Tris*(*dimethylamino*)*phosphazene*. P,P,P-*Tris*(*dimethylamino*)*iminophosphorane*
[49778-01-0]

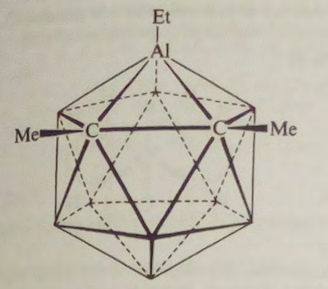
$$(Me_2N)_3P{=}NH$$

M 178.2
Liq. Bp_{10} 96-97°, $Bp_{0.1}$ 60-62°.
B, HCl: [87863-65-8]. N,N,N′,N′,N″,N″-*Hexamethyltetraaminophosphonium chloride*. *Aminotris*(*dimethylamino*)*phosphonium chloride*
$C_6H_{20}ClN_4P$ M 214.6
Cryst. (CH_2Cl_2/Et_2O). Mp 146-148°.
B, HBr: N,N,N′,N′,N″,N″-*Hexamethyltetraaminophosphonium bromide*. *Aminotris*(*dimethylamino*)*phosphonium bromide*
$C_6H_{20}BrN_4P$ M 259.1
Cryst. (CH_2Cl_2/Et_2O). Mp 185-186°.
N‴-*Chloro:* [78050-96-1].
$C_6H_{18}ClN_4P$ M 212.6
Undistillable, yellow mobile liq. Slowly dec. at 20°. Stable only in soln.

Issleib, K. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1973, **3**, 255 (*synth, pmr, P-31 nmr*)
Lorberth, J. *et al, J. Organomet. Chem.*, 1974, **71**, 159 (*synth, deriv*)
Egorov, Yu.P. *et al, Teor. Eksp. Khim.*, 1982, **18**, 58; *Theor. Exp. Chem. (Engl. Transl.)*, 1982, **18**, 45 (*P-31 nmr, struct*)
Egorov, Yu.P. *et al, Zh. Obshch. Khim.*, 1983, **53**, 2222; *J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 2003 (*ir, P-31 nmr*)
Marchenko, A.P. *et al, Zh. Obshch. Khim.*, 1983, **53**, 670; *J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 583 (*deriv, P-31 nmr*)

$C_6H_{20}AlB_9$ IC-005428

Ethyl](7,8,9,10,11-η)-1,2,3,4,5,6,9,10,11-nonahydro-7,8-dimethyl-7,8-dicarbaundecaborato(2−)]aluminium, 12Cl
2,3-Dimethyl-1-ethyl-1,2,3-aluminadicarbadodecaborane(*9*).
3-Ethyl-1,2-dimethyl-3-aluminio-1,2-dicarba-closo-*dodecaborane*(*12*)
[111908-13-5]



M 216.5
closo-. Reagent for synthesis of metal carbollides.
Colourless air- and moisture-sensitive solid. Mp 84-86°. $Bp_{0.01}$ 70°.

Et_2O complex: [111876-60-9]. *1-(Diethyl ether)-2,3-dimethyl-1-ethyl-1,2,3-aluminadicarbadodecaborane*(*9*)
$C_{10}H_{30}AlB_9O$ M 290.6
Colourless air- and moisture-sensitive needles. Mp 330° dec.

THF complex: [111876-61-0]. *2,3-Dimethyl-1-ethyl-1-tetrahydrofuran-1,2,3-aluminadicarbadodecaborane*(*9*)
$C_{10}H_{28}AlB_9O$ M 288.6
Colourless air- and moisture-sensitive needles. Mp 308° dec.

Jutzi, P. *et al, J. Organomet. Chem.*, 1987, **319**, 139 (*synth, pmr, cmr, B-11 nmr, Al-27 nmr*)

$C_6H_{20}BN_2^{\oplus}$ IC-005429

Dihydrobis(trimethylamine)boron(1+)
Bis(N,N-*dimethylmethanamine*)*dihydroboron*(*1+*), *10Cl*.
Bis(*trimethylamine*)*boronium*(*1+*)

$$[(Me_3N)_2BH_2]^{\oplus}$$

M 131.0 (ion)
Chloride: [18517-67-4].
$C_6H_{20}BClN_2$ M 166.5
No phys. props. reported.

Fr. Pat., 1 394 178, (1965); *CA*, **63**, 15897a.
Miller, N.E., *Inorg. Chem.*, 1977, **16**, 2664 (*synth*)
Miller, N.E., *J. Organomet. Chem.*, 1977, **137**, 131.

$C_6H_{20}B_{10}HgO$ IC-005430

[2-(Ethoxymethyl)-1,2-dicarbadodecaboran(12)-1-yl-*C,O*]methylmercury, 10Cl
(*Ethoxymethyl-o-carboranyl*)*methylmercury*.
Ethoxymethyl(*methylmercuri*)-o-*carborane*
[79374-09-7]

As Chloro(2-methyl-1,2-dicarbadodecaboran(12)-1-yl) mercury, IC-003727 with

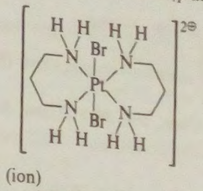
$$R^1 = -HgMe,\ R^2 = CH_2OEt$$

M 416.9
Cryst. (heptane). Mp 117-118°.

Yanovskii, A.I. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1981, **22**, 406 (*synth, cryst struct*)

$C_6H_{20}Br_2N_4Pt^{2\oplus}$ IC-005431

Dibromobis(1,3-propanediamine)platinum(2+), 9Cl
Dibromobis(*1,3-diaminopropane*)*platinum*(IV)



trans-form

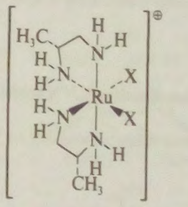
M 503.1 (ion)
Complexes of $[Pt(diamine)_2]^{2\oplus}$ have stacked structs. and 1-dimensional electric conductance. Cl and Pd analogues also known.

$[Pt(1,3\text{-propanediamine})_2]^{2\oplus}$ double salt, tetraperchlorate: [67758-24-1].
$C_{12}H_{40}Br_2Cl_4N_8O_{16}Pt_2$ M 1244.2
Dark green or green-gold dichroic needles; blue powder.
[87525-34-6]

Matsumoto, N. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 2334, 3514 (*synth, cryst struct*)
Yamashita, M. *et al, Inorg. Chim. Acta*, 1978, **31**, L381 (*pe*)
Clark, R.J.H. *et al, Inorg. Chem.*, 1980, **19**, 3522 (*raman, uv*)
Aoki, R. *et al, Mol. Cryst. Liq. Cryst.*, 1982, **81**, 301 (*elec cond*)

$C_6H_{20}Br_2N_4Ru^{\oplus}$ IC-005432

Dibromobis(*R*-1,2-propylenediamine)ruthenium(*III*)(1+)
Dibromobis(R-*1,2-diaminopropane*)*ruthenium*(III).
Dibromobis(R-*1,2-propanediamine*-N,N′)*ruthenium*(*1+*), *8Cl*



cis-form

X = Br

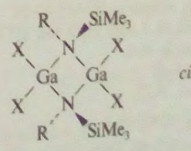
M 409.1 (ion)
Prepd. in same manner as the ethylenediamine analogue Dibromobis(ethylenediamine)ruthenium(*III*)(1+), IC-004332. Sol. H_2O.

Dibromide: [15406-36-7].
Red-brown solid.

Broomhead, J.A. *et al, J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv, hydration*)
Broomhead, J.A. *et al, Inorg. Chem.*, 1968, **7**, 2519 (*hydration*)

$C_6H_{20}Br_4Ga_2N_2Si_2$ IC-005433

Tetrabromobis(trimethylsilylamido)digallium
Tetrabromobis[*μ*-(*1,1,1-trimethylsilanaminato*)]*digallium, 12Cl*



cis-form

R = H, X = Br

M 635.4
cis and *trans* isomers in soln., *trans* in solid state. Synth. from $GaBr_3$ and $NH(SiMe_3)_2$.

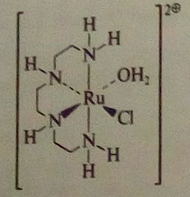
cis-form [120329-66-0]
Not isol., detected in soln. by nmr.

trans-form [120263-15-2]
Colourless air- and moisture-sensitive cryst. (Et_2O). Mp 170-172°.

Nutt, R.N. *et al, Inorg. Chem.*, 1989, **28**, 2224 (*pmr, Si-29 nmr, ir, synth, cryst struct*)

$C_6H_{20}ClN_4ORu^{2\oplus}$ IC-005434

Aquachloro(triethylenetetramine)ruthenium(*III*)(2+)
Aquachloro(1,8-diamino-3,6-diazaoctane)ruthenium(III)(*2+*)



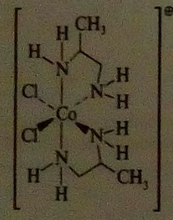
M 300.7 (ion)
Sol. H_2O.

4-Methylbenzenesulfonate: Tosylate
Prepd. by treating Dichloro(triethylenetetramine) ruthenium(*III*)(1+), IC-005324 with silver tosylate. Yellow cryst. + $1H_2O$.

Broomhead, J.A. *et al, Inorg. Chem.*, 1968, **7**, 2519 (*synth, equation*)

$C_6H_{20}Cl_2CoN_4^{\oplus}$ IC-005435

Dichlorobis(1,2-propanediamine-*N,N'*)cobalt(*III*)(1+), 1ICl
Dichlorobis(1,2-diaminopropane)cobalt(III)(*1+*)
[46139-68-8]



all-cis-form

M 278.0 (ion)

all-cis-form
Photolytic isom. occurs in MeOH.
Chloride: Hygroscopic purple solid. V. sol. H_2O.

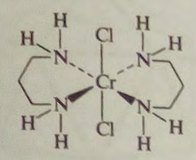
all-trans-form
Converts to *cis*-form > 80° in acid-free soln.
Chloride: [29990-94-1].
Green cryst. Sol. hot EtOH, MeOH.
Chloride, $HCl.(H_2O)_2$ complex: [50432-40-1].
Green solid. Sol. H_2O. Loses H_2O and HCl at 100° to afford the *cis*-chloride salt.
Perchlorate: [36673-00-4].
Green cryst. Sl. sol. H_2O.

[15041-15-3, 87465-05-2, 87465-06-3]

Werner, A. *et al, Ber.*, 1907, **40**, 2225.
Bailar, J.C. *et al, J. Am. Chem. Soc.*, 1939, **61**, 2402.
Martinette, M. *et al, J. Am. Chem. Soc.*, 1955, **77**, 6507 (*synth*)
Brasted, R.C., *J. Am. Chem. Soc.*, 1958, **80**, 788 (*isom*)
Haines, R.A. *et al, Can. J. Chem.*, 1971, **49**, 3907 (*synth*)
Le May, H.E., *Inorg. Chem.*, 1971, **10**, 1990 (*synth, trans-form*)
Le May, H.E. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 469 (*synth, uv-vis, cis-form*)
Hawkins, C.J. *et al, Aust. J. Chem.*, 1977, **30**, 2115 (*cd, pmr*)

$C_6H_{20}Cl_2CrN_4$ IC-005436

Dichlorobis(1,3-propanediamine)chromium(*II*), 8Cl
Dichlorobis(1,3-diaminopropane)chromium(II)
[33864-96-9]

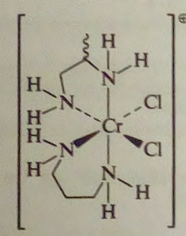


M 271.1
trans-Octahedral. Air-sensitive violet solid. $\mu_{eff} = 4.80\mu_B$ (90-300K). Corresp. bromide and iodide also known.

Larkworthy, L.F. *et al, J. Chem. Soc. A*, 1971, 2766 (*synth, props*)

$C_6H_{20}Cl_2CrN_4^{\oplus}$ IC-005437

Dichloro(1,2-propanediamine-*N,N'*)(1,3-propanediamine-*N,N'*)chromium(*III*)(1+), 11Cl, 10Cl



cis-form

M 271.1 (ion)
Approx. octahedral cation.

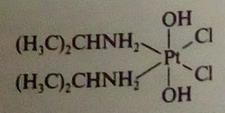
cis-form
Chloride: [81244-80-6].
Violet cryst.

trans-form
Chloride: [71861-02-4].
Green cryst. + H_2O. Dehydrates at 40-120°. Dec. during isomerisation at ~220°.

Mitra, S. *et al, Bull. Chem. Soc. Jpn.*, 1979, **52**, 2569 (*synth, dec*)
Uehara, A. *et al, Inorg. Chem.*, 1982, **21**, 2422 (*synth*)

$C_6H_{20}Cl_2N_2O_2Pt$ IC-005438

Iproplatin, BAN, USAN, INN
Dichlorodihydroxybis(2-propanamine)platinum, 9CI. ab-
Dichloro-ce-dihydroxy-df-bis(isopropylamine)platinum(IV).
Dichlorodihydroxybis(2-propanamine)platinum, 11CI. CHIP. JM 9. NSC 256927
[62928-11-4]



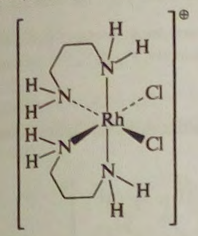
M 418.2
Antineoplastic agent. Yellow cryst. + $\frac{1}{2}$ H_2O (H_2O). Sol. H_2O.

▷ TP2494300.
[83291-20-7, 89673-10-9, 97101-53-6]

Connors, T.A. *et al, Chem. Biol. Interact.*, 1972, **5**, 415.
Tobe, M.L. *et al, J. Clin. Hematol. Oncol.*, 1977, **7**, 114 (*pharmacol*)
U.K. Pat., 1 578 323, (1980); *CA*, **87**, 177982u (*synth*)
Laverick, M. *et al, Br. J. Radiol.*, 1981, **54**, 529 (*pharmacol*)
Pendyala, L. *et al, Cancer Treat. Rep.*, 1982, **66**, 509 (*metab*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 18653.
Barnard, C.F.J. *et al, J. Chem. Res. (S)*, 1983, **12**, 302 (*synth, cryst struct, raman*)
Brandon, R.J. *et al, J. Med. Chem.*, 1984, **27**, 861 (*Pt-195 nmr*)
Harrap, K.R., *Cancer Treat. Rep.*, 1985, **12A**, 21 (*rev*)
Chang, P., *Drugs of the Future*, 1985, **10**, 561 (*rev*)
Barnard, C.F.J. *et al, Chem. Ber.*, 1986, **22**, 1001 (*rev*)

$C_6H_{20}Cl_2N_4Rh^{\oplus}$ IC-005439

Dichlorobis(1,3-propanediamine-*N,N'*)rhodium(*III*)(1+), 10Cl
Dichlorobis(trimethylenediamine)rhodium(III)



cis-form

M 322.0 (ion)

cis-form [65437-15-2]
Perchlorate: [65437-16-3].
Lemon-yellow cryst. +$2H_2O$ (hot H_2O). Sol. H_2O.

trans-form [52795-66-1]
Chloride: [92186-50-0].
Yellow solid.
Perchlorate: [65394-33-4].
Long orange needles (70% $HClO_4$). Sol. H_2O.

Johnson, S.A., *Inorg. Chem.*, 1962, **1**, 925 (*synth, uv*)
Johnson, S.A., *J. Am. Chem. Soc.*, 1963, **85**, 1741.
Hancock, M.P., *Acta Chem. Scand., Ser. A*, 1977, **31**, 678 (*synth, perchlorate, uv*)

$C_6H_{20}Cl_2N_4Ru^{\oplus}$ IC-005440

Dichlorobis(*R*-1,2-propanediamine-*N,N'*)ruthenium(1+), 8Cl
Dichlorobis(R-*1,2-diaminopropane*)*ruthenium*(III).
Dichlorobis(R-*1,2-propylenediamine*)*ruthenium*(III)(*1+*)
As Dibromobis(*R*-1,2-propylenediamine)ruthenium(*III*) (1+), IC-005432 with

X = Cl

M 320.2 (ion)
Prepd. analogously to the ethylenediamine analogue, Dichlorobis(ethylenediamine)ruthenium(1+), IC-004357. Sol. H_2O.

Chloride: [15406-35-6].
Yellow salt. Ir ν_{RuCl} 324, 276 cm^{-1}.

Broomhead, J.A. *et al, J. Chem. Soc. A*, 1967, 546 (*synth, ir, uv*)
Broomhead, J.A. *et al, Inorg. Chem.*, 1968, **7**, 2519 (*hydration*)

$C_6H_{20}Cl_4Ga_2N_2Si_2$ IC-005441

Tetrachlorobis(trimethylsilylamido)digallium
Tetrachlorobis[μ-(1,1,1-trimethylsilanaminato)]digallium, 11CI

As Tetrabromobis(trimethylsilylamido)digallium, IC-005433 with

R = H, X = Cl

M 457.6
Synth. from $GaCl_3$ and $(Me_3Si)_2NH$.

cis-form [93779-96-5]
Not isol. Detected in soln. by nmr.

trans-form [93779-95-4]
Colourless air and moisture sensitive solid (CH_2Cl_2). Sol. CH_2Cl_2, toluene. Mp 157-158°. A *trans* trimer has also been detected in soln. ($C_9H_{30}Cl_6Ga_3N_3Si_3$).

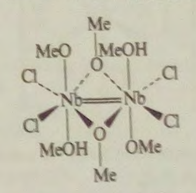
Monomer: Dichloro(trimethylsilylamido)gallium.
Trimethylsilylgallium dichloride.
Dichloro(trimethylsilylamino)gallane
$C_3H_{10}Cl_2GaNSi$ M 228.8
Not yet descr.

[93714-41-1]

Wiberg, N. *et al, Z. Anorg. Allg. Chem.*, 1966, **345**, 93 (*synth*)
Nutt, W.R. *et al, Inorg. Chem.*, 1985, **24**, 159 (*synth, pmr, cmr, Si-29 nmr, ir, cryst struct*)

$C_6H_{20}Cl_4Nb_2O_6$ IC-005442

Tetrachlorobis(methanol)di-μ-methoxydimethoxydiniobium(*IV*), 11Cl
Di-μ-methoxobis[dichloro(methoxy)(methanol)niobium(IV)]
[98394-03-7]

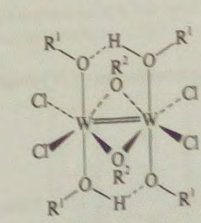


M 515.8
Synth. from Nb_2Cl_6(tetrahydrothiophene)$_3$ and MeOH in THF. Minor product. Dark blue solid.

Cotton, F.A. *et al, Inorg. Chem.*, 1985, **24**, 3509 (*synth, cryst struct*)

$C_6H_{20}Cl_4O_6W_2$ IC-005443

Tetrachlorobis(methanol)di-μ-methoxydimethoxyditungsten(*IV*), 10Cl
[78338-25-7]



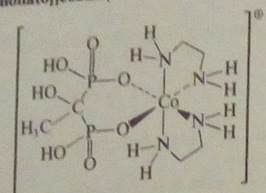
$R^1 = R^2 = Me$

M 697.7
2 Distorted octahedra sharing an edge. Formal W=W 248.1, W—Cl_{av} 238.6 pm. Dark green cryst. (MeOH).

Anderson, L.B. *et al, J. Am. Chem. Soc.*, 1981, **103**, 5078 (*cryst struct, electrochem, synth*)

$C_6H_{22}CoN_4O_7P_2^{\oplus}$ IC-005444

Bis(ethylenediamine)[(1-hydroxyethylidene)bis[phosphonato]]cobalt(1+)



M 381.1 (ion)
Complexes with $Ca^{2\oplus}$ in H_2O.
Perchlorate: [84895-57-8].
Red cryst. + $2H_2O$. Sol. H_2O.

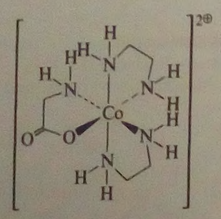
[84895-44-3]

Jurisson, S.S. *et al, Inorg. Chem.*, 1983, **22**, 1332 (*synth, pmr, P-31 nmr, cryst struct*)

$C_6H_{20}CoN_5O_2^{2\oplus}$ IC-005445

Bis(ethylenediamine)glycinatocobalt(*III*)(2+)
*Bis(1,2-ethanediamine-*N,N′*)(glycinato-*N,O*)cobalt*(III)(2+), *9CI*

[16070-98-7]



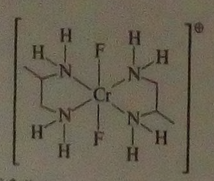
M 253.1 (ion)
Implicated in peptide bond formn. in non aq. solvs.
Dichloride: [14408-57-2].
Orange solid + $2H_2O$.

[19657-79-5, 19657-80-8, 54003-28-0]

Lin, T.C. *et al, Inorg. Chem.*, 1964, **3**, 1356 (*synth*)
Alexander, M.D. *et al, Inorg. Chem.*, 1966, **5**, 1590 (*synth*)
Buckingham, D.A. *et al, J. Am. Chem. Soc.*, 1967, **89**, 4539 (*reaction*)
Meisenheimer, J., *Justus Liebigs Ann. Chem.*, 1974, **438**, 217 (*synth, resoln*)
Lane, R.H. *et al, Inorg. Chem.*, 1977, **16**, 93 (*synth, uv-vis, ir, pmr*)
Harrison, R.G. *et al, J. Chem. Educ.*, 1982, **59**, 1054 (*synth, ir, uv-vis*)

$C_6H_{20}CrF_2N_4^{\oplus}$ IC-005446

Difluorobis(1,2-propanediamine-*N,N′*)chromium(*III*)(1+), 11CI, 9CI



trans-form

M 238.2 (ion)

cis-form
More sol. than *trans*-form.
Bromide: [40902-44-1].
Pink solid. Sol. EtOH.
Tetraphenylborate: [49634-00-6].
Pink solid + 1.5 H_2O (MeOH/Et_2O).

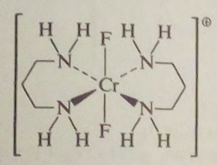
trans-form
(±)-*form*
Bromide: [40902-40-7].
Pink-orange solid + H_2O. Insol. EtOH.
Perchlorate: [27783-40-0].
Orange-red solid or light red needles + $2H_2O$.
Tetrafluoro(1,2-propanediamine)chromate(III): see *Tetrafluoro(1,2-propanediamine-*N,N′*)chromate*(III)(*1−*), *IC-003709*

(+)-*trans-form*
Synth. using (−)-1,2-propanediamine.
Perchlorate: [27712-12-5].
Solid.

Glerup, J. *et al, Acta Chem. Scand.*, 1970, **24**, 247 ((+)-*form, synth*)
Vaughn, J.W. *et al, Inorg. Chem.*, 1973, **12**, 2346; 1974, **13**, 598 (*synth, uv-vis*)
Kaizaki, S., *Bull. Chem. Soc. Jpn.*, 1983, **56**, 3620 (*cd*, (+)-*form, uv-vis*)
Casabó, J. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1983, **13**, 835 (*synth*)

$C_6H_{20}CrF_2N_4^{\oplus}$ IC-005447

Difluorobis(1,3-propanediamine-*N,N′*)chromium(*III*)(1+), 11CI, 10CI, 9CI



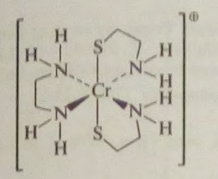
M 238.2 (ion)
Octahedral cation. Acid hydrol. produces *trans*-[Cr(1,3-propanediamine)F(H_2O)]$^{2\oplus}$.

trans-form [42476-30-2]
Both rings (Cr-amine) are in chair conformn. Cr-N_{av} 208.5, Cr-F_{av} 187.6 pm.
Chloride: [63231-42-5].
Cryst. + H_2O (aq. HCl).
Perchlorate: [27712-11-4].
Bright red needles.
▷ Potentially explosive.

Glerup, J. *et al, Acta Chem. Scand.*, 1970, **24**, 247 (*synth, perchlorate*)
Vaughn, J.W. *et al, Inorg. Chem.*, 1970, **9**, 2786 (*synth*)
Vaughn, J.W. *et al, J. Crystallogr. Spectrosc. Res.*, 1985, **15**, 281 (*cryst struct, perchlorate*)
Kirk, A.D. *et al, Inorg. Chem.*, 1986, **25**, 2225 (*photochem, acid hydrol, chloride*)

$C_6H_{20}CrN_4S_2^{\oplus}$ IC-005448

Bis(2-aminoethanethiolato-*N,S*)(1,2-ethanediamine-*N,N′*)chromium(*III*)(1+), 9CI
Ethylenediaminebis(2-mercaptoethylamine)chromium(III)(*1+*)



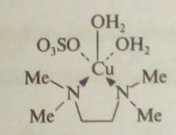
M 264.3 (ion)
Approx. octahedral geometry, with *trans*-S atoms.
Perchlorate: [41777-29-1].
Red or violet cryst. (H_2O).

Weschler, C.J. *et al, Inorg. Chem.*, 1973, **12**, 2682 (*synth*)
Stein, C. *et al, Inorg. Chem.*, 1976, **15**, 1183 (*cryst struct, synth*)

$C_6H_{20}CuN_2O_6S$ IC-005449

Diaquasulfato(*N,N,N′,N′*-tetramethylethylenediamine)copper(*II*)
*Diaqua[sulfato(2−)-*O*](*N,N,N′,N′*-tetramethyl-1,2-ethanediamine-*N,N′*)copper*(II), *9CI*

[57196-94-8]



M 311.8
Tetragonal pyramidal geometry. Light blue powder. Sol. H_2O; insol. Et_2O. μ_{eff} = 1.87μ_B.

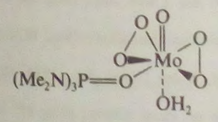
[106062-67-3]

Balvich, J. *et al, Inorg. Chem.*, 1976, **15**, 71 (*synth, cryst struct, ir*)
Pisipati, V.G.K.M. *et al, Org. Magn. Reson.*, 1984, **22**, 629 (*esr*)
Muralikrishna, V. *et al, Indian J. Pure Appl. Phys.*, 1986, **24**, 358; 1988, **26**, 330 (*esr*)

$C_6H_{20}MoN_3O_7P$ IC-005450

Aqua(hexamethylphosphoric triamide-*O*)oxodiperoxymolybdenum, 9CI
Oxodiperoxo(hexamethylphosphoramide)aquomolybdenum(VI)

[23319-56-4]



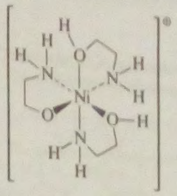
M 373.1
Pentagonal bipyramidal complex; analogous Py adduct known. Yellow cryst. (MeOH).

[36671-04-2]

Mimoun, H. *et al, Bull. Soc. Chim. Fr.*, 1969, 1481 (*synth, ir*)
Carpentier, J.-M.L. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 1278 (*cryst struct*)
Daniewski, A.R., *Synth. Commun.*, 1986, **16**, 535 (*synth*)

$C_6H_{20}N_3NiO_3^{\oplus}$ IC-005451

Bis(2-aminoethanol-*N,O*)(2-aminoethanolato-*N,O*)nickel(*II*)(1+)



M 240.9 (ion)
Octahedral at Ni.
Perchlorate: [70748-79-7].
Blue octahedral cryst. Sol. EtOH. μ_{eff} = 3.16μ_B (298K) 3.04μ_B (93K). Octahedral tris-chelates are formed face to face by hydrogen bonding.

Kida, S., *Nippon Kagaku Zasshi* (*Jpn. J. Chem.*), 1964, **85**, 32 (*synth*)
Bertrand, J.A. *et al, Inorg. Chem.*, 1979, **18**, 2419 (*synth, cryst struct*)

$C_6H_{20}N_4Ni^{2\oplus}$ IC-005452

Bis(1,2-propanediamine)nickel(*II*)(2+), 9CI
Bis(1,2-diaminopropane)nickel(II)(*2+*). *Bis(1,2-propylenediamine)nickel*(II)(2+)

[20037-68-7]

As Bis(ethylenediamine)nickel(*II*)(2+), IC-004376 with

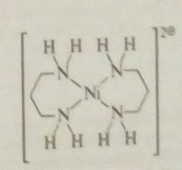
R = CH_3

M 206.9 (ion)
Square planar struct., solvs. may coordinate in solns. of simple salts.
Diperchlorate: [31381-62-1].
$C_6H_{20}Cl_2N_4NiO_8$ M 405.8
Yellow solid.
▷ Potentially explosive.
Chloride, compd. with Dichlorobis(1,2-propanediamine)nickel(2+): see [*Dichlorobis(1,2-propanediamine)nickel(2+)*][*bis(1,2-propanediamine)nickel(2+)*], *IC-008334*
Lifschitz, F. *et al, Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1941, **60**, 581 (*synth*)
Sone, K. *et al, Z. Anorg. Allg. Chem.*, 1959, **301**, 277 (*uv*)
Nishida, Y. *et al, Bull. Chem. Soc. Jpn.*, 1970, **43**, 3814 (*uv, esr*)

$C_6H_{20}N_4Ni^{2\oplus}$ IC-005453

Bis(1,3-propanediamine-*N,N′*)nickel(*II*)(2+)
Bis(1,3-diaminopropane)nickel(II)(*2+*), *8CI*

[55528-16-0]



M 206.9 (ion)
Dichloride: [15522-56-2].
$C_6H_{20}Cl_2N_4Ni$ M 277.8
Perchlorate, anhydrous: [49727-54-0].
$C_6H_{20}Cl_2N_4NiO_8$ M 405.8
Corresp. dihydrate is octahedral with coordn. by $2H_2O$.

▷ Potentially explosive.

[24419-44-1]

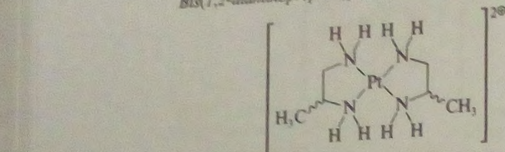
Pajunen, A., *Suom. Kem. B*, 1969, **42**, 397.

IC-005454

$C_6H_{20}N_4Pt^{2\oplus}$

Bis(1,2-propanediamine-N,N')platinum(2+), 9CI

Bis(1,2-diaminopropane)platinum(II), *8CI*



M 343.3 (ion)

In cryst., rings have different conformation; in soln. conformations rapidly interconvert. Also forms 1:1:4 salts with $[Pt(diamine)_2X_2]^{2\oplus}$ and $Y^{\ominus}$ (see Pt (*IV*) sp.).

Dichloride: [17830-46-5].
$C_6H_{20}Cl_2N_4Pt$ M 414.2
White solid. Sol. H_2O.

Dichloride, dihydrate: [74497-51-1].
Colourless cryst. Sol. H_2O.

[58410-55-2]

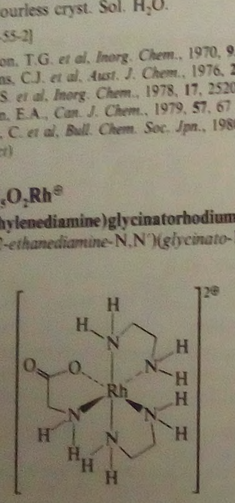
Appleton, T.G. *et al*, *Inorg. Chem.*, 1970, **9**, 1800 (*synth*)
Hawkins, C.J. *et al*, *Aust. J. Chem.*, 1976, **29**, 33 (*pmr*)
Yano, S. *et al*, *Inorg. Chem.*, 1978, **17**, 2520 (*synth, pmr, cmr*)
Sullivan, E.A., *Can. J. Chem.*, 1979, **57**, 67 (*uv-vis, cd*)
Maeda, C. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 1755 (*cryst struct*)

IC-005455

$C_6H_{20}N_5O_2Rh^{\oplus}$

Bis(ethylenediamine)glycinatorhodium(*III*)(2+)

Bis(1,2-ethanediamine-N,N')(glycinato-N,O)rhodium(2+), 9CI



Δ-form

M 297.1 (ion)

Optically active amino acid complex. Mod. stable in soln.

Δ-form

(+)-form

Diiodide: $[\alpha]_D$ +39°.

Λ-form

(−)-form

Diiodide: $[\alpha]_D$ −39°.

(±)-form

Diiodide: [14896-61-8].
Synth. from *trans*-$[Rh(en)_2Cl_2]NO_3$, glycine, NaOH and a trace of EtOH. Cream-coloured cryst. (hot H_2O).

Dithionate: [52729-91-6].
White solid.

Waller, J.F. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 2371 (*synth*)
Hall, S.K. *et al*, *Inorg. Chem.*, 1968, **7**, 530 (*synth, cd, resoln*)
Addison, S.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 709 (*synth, dithionate*)

$C_6H_{20}N_5RuS^{2\oplus}$

IC-005456

Pentaammine(phenylthio)ruthenium(*III*)(2+)

Pentaammine(benzenethiolato)ruthenium(III)(2+)

$[Ru(NH_3)_5SPh]^{2\oplus}$

M 295.3 (ion)

Pseudo-octahedral. Prepd. by treating Pentaammine(aqua) ruthenium(*II*)(2+), IC-019980 with S_2Ph_2, or with PhSH followed by aerial oxidation. Sol. H_2O, Me_2CO.

Bis-hexafluorophosphate: [70288-23-2].
Red salt.

Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 2212 (*synth, uv*)

$C_6H_{20}N_5RuSe^{2\oplus}$

IC-005457

Pentaammine(phenylseleno)ruthenium(*III*)(2+)

Pentaammine(benzeneselenato)ruthenium(III)(2+)

$[Ru(NH_3)_5SePh]^{2\oplus}$

M 342.2 (ion)

Pseudo-octahedral. Prepd. by heating Pentaammine(aqua) ruthenium(*II*)(2+), IC-019980 with Se_2Ph_2. Sol. H_2O, Me_2CO.

Bis-hexafluorophosphate: [70288-25-4].
Blue salt.

Stein, C.A. *et al*, *Inorg. Chem.*, 1979, **18**, 2212 (*synth, uv*)

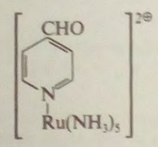
$C_6H_{20}N_6ORu^{2\oplus}$

IC-005458

Pentaammine(4-pyridinecarboxaldehyde-N^1) ruthenium(*III*)(2+), 9CI

Pentaammine(pyridine-4-aldehyde)ruthenium(II)(2+)

[19471-56-8]



M 293.3 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with pyridine-4-aldehyde. Sol. H_2O. In equilibrium with Pentaammine(4-pyridinylmethanediol-*N*)ruthenium(2+), IC-005482 in H_2O, with over 90% in the non-hydrated form (cf. Pentaammine(4-pyridinecarboxaldehyde-N^1)ruthenium(3+), IC-005460).

Dibromide:

Bis-tetrafluoroborate:

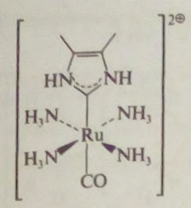
Ford, P. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 1187 (*synth, uv, electrochem*)
Zanella, A.W. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 7166 (*synth, uv, equilm*)
Malouf, G. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 601; 1977, **99**, 7213 (*photochem*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*electrochem, uv*)
Okano, V. *et al*, *J. Org. Chem.*, 1981, **46**, 1018 (*hydration*)
Benedix, R. *et al*, *J. Prakt. Chem.*, 1984, **326**, 962 (*uv, photochem, theory*)

IC-005459

$C_6H_{20}N_6ORu^{2\oplus}$

Tetraamminecarbonyl(1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene)ruthenium(2+), 9CI

Tetraammine(carbonyl)(4,5-dimethylimidazole)ruthenium(II)(2+)



M 293.3 (ion)

The imidazole ligand is bound through C(2) as an ylid; *trans*- octahedral at Ru Ru—N 213.6, Ru—$C_{im.}$ 212.8; Ru—C 184.9 pm. Prepd. by reducing Tetraamminechloro(1,3-dihydro-4,5-dimethyl-2*H*-imidazol-2-ylidene)ruthenium(2+), IC-004797 with Zn/Hg, followed by CO. Sol. H_2O, DMSO, Me_2CO.

Bis-hexafluorophosphate: [52125-02-7].
Cryst. + 1DMSO (DMSO then Me_2CO).

Sundberg, R.J. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 381 (*synth, pmr, uv, electrochem, cryst struct*)

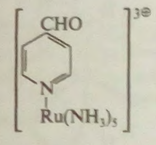
IC-005460

$C_6H_{20}N_6ORu^{3\oplus}$

Pentaammine(4-pyridinecarboxaldehyde-N^1) ruthenium(3+), 9CI

Pentaammine(pyridine-4-aldehyde)ruthenium(III)(3+)

[35419-53-5]



M 293.3 (ion)

Minor species in equilibrium with a hydrated form, $[Ru(NH_3)_5[NC_5H_4CH(OH)_2]]^{3\oplus}$. Prepd. in soln. by oxidation of Pentaammine(4-pyridinecarboxaldehyde-*N*) ruthenium(*III*)(2+), IC-005458. Not isol. Sol. H_2O.

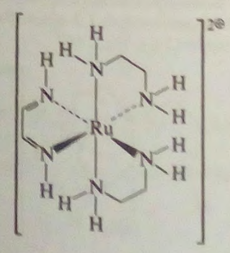
Zanella, A.W. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 7166 (*synth, hydration*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*synth, electrochem*)

IC-005461

$C_6H_{20}N_6Ru^{2\oplus}$

(Ethanediimine-N,N')bis(ethylenediamine-N,N') ruthenium(*II*)(2+)

Bis(1,2-ethanediamine-N,N')(ethanediimine-N,N') ruthenium(2+), 9CI



M 277.3 (ion)

Originally misformulated as a ruthenium(*VI*) salt. Prepd. by oxidizing Tris(ethylenediamine)ruthenium(*II*)(2+), IC-005518 or Tris(ethylenediamine)ruthenium(3+), IC-005519 with I_2 or O_2.

Diiodide: [36216-30-5].
Brown salt.

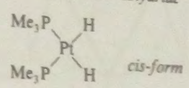
Lane, B.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 1618 (*synth, pe, pmr*)
Mahoney, D.F. *et al*, *Inorg. Chem.*, 1973, **12**, 2561 (*synth, uv, pmr, electrochem*)
Seddon, E.A. *et al*, *The Chemistry of Ruthenium*, Elsevier, Amsterdam, 1984, 74, 259, 289 (*rev*)

IC-005462

$C_6H_{20}P_2Pt$

Dihydrobis(trimethylphosphine)platinum

Bis(trimethylphosphine)platinum dihydride



cis-form

M 349.2

Rapid *cis-trans* isomerism obs. in soln.

▷ Pyrophoric.

cis-form [80540-35-8]
Not isol. Ir ν_{Pt-H} 2030, 1985 cm^{-1}. Readily dec. by H_2 loss in soln., but stable under H_2 atm.

trans-form [80581-71-1]
Cryst. + 1 naphthalene (THF). Ir ν_{Pt-H} 1720 cm^{-1}. Readily loses H_2 in soln., but stable under H_2 atm.

Packett, D.L. *et al*, *Inorg. Chem.*, 1985, **24**, 3578 (*synth, struct, pmr, P-31 nmr*)
Packett, D.L. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 5036 (*synth, ir*)

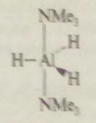
IC-005463

$C_6H_{21}AlN_2$

Trihydrobis(trimethylamine)aluminium

Bis(trimethylamine)alane. Aluminium hydride bis(trimethylamine)

[17211-58-4]



M 148.2

Trigonal pyramidal at Al. Synth. from Me_3NAlH_3 + Me_3N. Mp 95°.

Ruff, J.K. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 2141 (*synth*)
Heitsch, C.W. *et al*, *Inorg. Chem.*, 1963, **2**, 508 (*synth, cryst struct*)
Fraser, G.W. *et al*, *J. Chem. Soc.*, 1963, 3742 (*synth, ir, raman*)
Heitsch, C.W. *et al*, *Spectrochim. Acta*, 1963, **19**, 1385 (*ir, raman*)
Rosinski, H. *et al*, *Z. Phys. Chem. (Munich)*, 1963, **36**, 26 (*ir*)
Beattie, I.R. *et al*, *J. Chem. Soc.*, 1964, 3528 (*ir, raman*)

IC-005464

$C_6H_{21}BN_3P$

(Hexamethylphosphorous triamide)trihydroboron, 10CI

Hexamethylphosphorous triamide compd. with borane (1:1), 9CI, 8CI. Borane tris(dimethylamino)phosphine. Hexamethylphosphorous triamide borine

[7319-05-3]

$(Me_2N)_3P{-}BH_3$

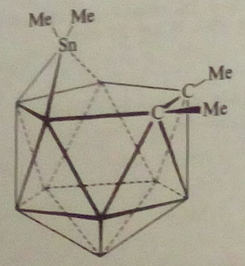
M 177.0

Cryst. with camphoraceous odour. Mp 32.5°. Bp 49-50°.

Reetz, T. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 5036 (*synth*)
Laurent, J.P. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 26.
Laurant, J.P. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 1353 (*nmr*)
Cowley, A.H. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 6815 (*pmr, nmr*)
Jouany, C. *et al*, *Bull. Soc. Chim. Fr.*, 1972, 880 (*pmr, nmr*)
Elegant, L. *et al*, *Can. J. Chem.*, 1978, **56**, 857 (*pmr, nmr*)

IC-005465

$C_6H_{21}B_9Sn$
1,1,2,3-Tetramethyl-1-stanna-2,3-dicarbadodecaborane(9)
[111867-42-6]



M 309.2
nido-. Colourless cryst. ($CHCl_3$). Mp 198-203° dec.
Jutzi, P. *et al*, *J. Organomet. Chem.*, 1987, **319**, 139 (*synth, pmr, cmr, B-11 nmr, Sn-119 nmr, ms*)

IC-005466

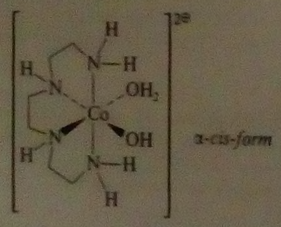
$C_6H_{21}ClCrN_5^{2\oplus}$
Chloro(diethylenetriamine)(ethylenediamine)chromium(*III*)(2+)
[N-(2-Aminoethyl)-1,2-ethanediamine-N,N′,N″]chloro(1,2-ethanediamine-N,N′)chromium(2+), 9Cl. Chloro(1,5-diamino-3-azapentane)(1,2-diaminoethane)chromium(III) (2+)
[59184-05-3]

$[CrCl(H_2NCH_2CH_2NH_2)(H_2NCH_2CH_2NHCH_2CH_2NH_2)]^{2\oplus}$

M 250.7 (ion)
Octahedral, but detailed stereochem. not reported.
Tetrachlorozincate(2−): [59184-06-4].
Synth. from $CrCl_3.6H_2O$ + nitrogen ligands in DMSO with $ZnCl_2$ to provide counter ion. Orange-red cryst. λ_{max} 373, 514 nm.
House, D.A., *Inorg. Nucl. Chem. Lett.*, 1976, **12**, 259 (*synth, kinetics, powder struct, us-cis*)
Dawson, B.S. *et al*, *Inorg. Chem.*, 1977, **16**, 1354 (*kinetics*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 806 (*rev*)

IC-005467

$C_6H_{21}CoN_4O_2^{2\oplus}$
Aquahydroxy(triethylenetetramine)cobalt(*III*)(2+)
Aquahydroxy(1,4,7,10-tetraazadecane)cobalt(III)(2+)



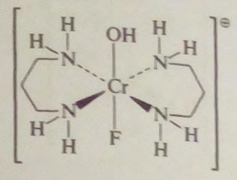
α-*cis-form*

M 240.1 (ion)

Used in hydrolysis of amino acid esters, peptides etc.
Obtd. in soln.
Buckingham, D.A. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 1082 (*synth*)

IC-005468

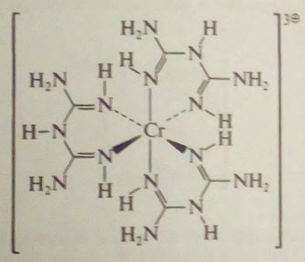
$C_6H_{21}CrFN_4O^{\oplus}$
Fluorohydroxybis(1,3-propanediamine-*N,N′*)chromium(*III*)(1+), 11Cl



M 236.2 (ion)
trans-Octahedral cation.
*Aquafluorobis(1,3-propanediamine-*N,N′*)chromium(2+) perchlorate (1:1:3)*: [85826-85-3].
Cryst. Struct. consists of complex cations linked by strong hydrogen bonds in infinite chains.
Solans, X. *et al*, *Cryst. Struct. Commun.*, 1982, **11**, 1199 (*cryst struct*)

IC-005469

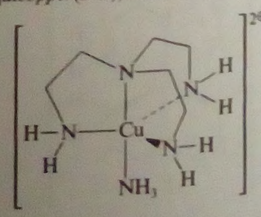
$C_6H_{21}CrN_{15}^{3\oplus}$
Tris(biguanide)chromium(*III*)(3+)
*Tris(imidodicarbonimidic diamide-*N″,N‴*)chromium*(III) *(3+), 10Cl, 9Cl*
[65929-21-7]



M 355.3 (ion)
Trichloride: [12152-13-5].
μ_{eff} = 3.88μ_B (278K).
Brubaker, G.R. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 7199 (*abs config*)
Kaizaki, S. *et al*, *Inorg. Chem.*, 1973, **12**, 142 (*cd*)
Pradham, B. *et al*, *J. Indian Chem. Soc.*, 1977, **54**, 127 (*props*)
Kurotaki, K. *et al*, *J. Chem. Soc., Faraday Trans. 1*, 1981, **77**, 217 (*props*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 850 (*rev*)

IC-005470

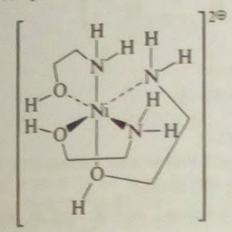
$C_6H_{21}CuN_5^{2\oplus}$
Ammine[tris(2-aminoethyl)amine]copper(*II*)(2+)
Ammine[N,N-*bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*dicopper(2+), 10Cl, 9Cl*



M 226.8 (ion)
Trigonal bipyramidal cation.
Diperchlorate: [75094-49-4].
Bright blue cryst.
▷ Potentially explosive.
Bis-tetraphenylborate: [54689-14-4].
Dark blue cryst. Insol. H_2O. Mp 124° dec. μ_{eff} = 1.9-2.2μ_B.
Albertin, G. *et al*, *Inorg. Chem.*, 1975, **14**, 1411 (*synth, props*)
Duggan, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1342 (*cryst struct, esr, us*)
Kurodu, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 2565 (*cd, ord*)
Deeth, R.J. *et al*, *Inorg. Chem.*, 1985, **24**, 4490.

IC-005471

$C_6H_{21}N_3NiO_3^{2\oplus}$
Tris(2-aminoethanol-*N,O*)nickel(*II*)(2+), 9Cl
[16969-78-1]



fac-form

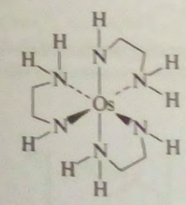
M 241.9 (ion)
Octahedral struct., *fac*-isomer in solid state.

fac-form
Nitrate: [31219-72-4].
Sulfate: [31219-73-5].
Diiodide, double complex with $[Co(NH_2CH_2CH_2O)_3]$:
$C_{12}H_{39}CoI_2N_6NiO_6$ M 734.9
Cubic cryst. Alcoholic H hydrogen bonds with O on Co complex. μ_{eff} = 3.12 μ_B. Paramagnetic Ni(*II*), diamagnetic Co(*III*).

mer-form
Nitrate: [31249-25-9].
Sulfate: [31249-26-0].
Bertrand, J.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 437 (*cryst struct*)

IC-005472

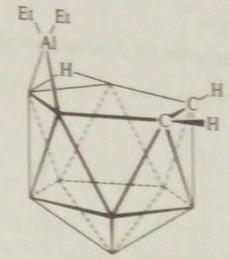
$C_6H_{21}N_6Os$
Tris(2-aminoethylamido)osmium(*III*)
Tris(1,2-ethanediaminato)osmium(III)
[15558-29-9]



M 367.4
Synth. from $[Os(en)_3]I_3$ and $3KNH_2$ in liq. NH_3. Moisture-sensitive brown solid.
Watt, G.W. *et al*, *Inorg. Chem.*, 1966, **5**, 857 (*synth, ir*)

IC-005473

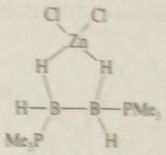
$C_6H_{22}AlB_9$
[Dodecahydro-7,8-dicarbaundecaborato(1−)-*H*^{8},*H*^{9,10}]diethylaluminium
7,8-μ-Diethylaluminio-1,2-dicarba-nido-undecaborane(13)
[11098-58-1]



M 218.5
Fluxional H spanning open face postulated. Colourless cryst. (hexane). Mp 34.5-35.5°.
▷ Explodes with water.
Young, D.A.T. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5687 (*synth, ir, pmr, nmr*)

IC-005474

$C_6H_{22}B_2Cl_2P_2Zn$
[1,2-Bis(trimethylphosphine)diborane(4)-*H*^{4},*H*$^{4'}$]dichlorozinc, 11Cl
[88730-79-4]



M 314.1
Colourless air-sensitive solid (Et_2O). Sol. CH_2Cl_2.
Kodama, G. *et al*, *Inorg. Chem.*, 1984, **23**, 511 (*synth, deriv, cryst struct, B-11 nmr, P-31 nmr, pmr*)

IC-005475

$C_6H_{22}B_2N_2$
Hexahydro[μ-(*N,N,N′,N′*-tetramethyl-1,2-ethanediamine-*N:N′*)]diboron, 10Cl
Tetramethylethylenediamine bis(borane). N,N,N′,N′-Tetramethyl-1,2-ethanediamine, compd. with borane (1:2), 9Cl
[5843-33-4]

$H_3B{-}Me_2NCH_2CH_2NMe_2{-}BH_3$

M 143.8
White solid. Mp 181-183°.
Miller, N.E. *et al*, *Inorg. Chem.*, 1964, **3**, 886.
Miller, H.C. *et al*, *Inorg. Chem.*, 1964, **3**, 1458 (*synth*)
Gatti, A.R. *et al*, *Inorg. Chem.*, 1966, **5**, 329 (*synth, pmr, nmr*)
Nainan, K.C. *et al*, *Inorg. Chem.*, 1969, **8**, 2671 (*synth, pmr, nmr*)
Hu, M.G. *et al*, *Inorg. Chim. Acta*, 1974, **10**, 83.
Brown, H.C. *et al*, *Inorg. Chem.*, 1980, **19**, 455.

IC-005476

$C_6H_{22}B_2P_2$
1,2-Bis(trimethylphosphine)tetrahydrodiborane(4), 10Cl
Diborane(4) compd. with trimethylphosphine (1:2)
[67113-98-8]

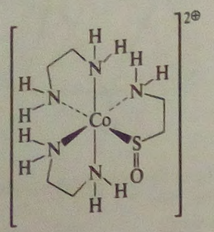
$(Me_3P)BH_2BH_2(PMe_3)$

M 177.8
Moisture sensitive colourless cryst. Sol. toluene, CCl_4. Mp 100° (sealed tube). Slowly dec. at r.t. *in vacuo*.

Hertz, R.K. *et al*, *Inorg. Chem.*, 1978, **17**, 2673 (*synth, ir, pmr, B-11 nmr, cmr, P-31 nmr*)

$C_6H_{22}CoN_5OS^{3\oplus}$ IC-005477

[(2-Aminoethyl)sulfinyl-*N,S*]bis(ethanediamine-*N,N'*)cobalt(*III*)(2+)
2-Aminoethanesulfenatobis(ethylenediamine)cobalt(III)(*2+*)
[68645-75-0]

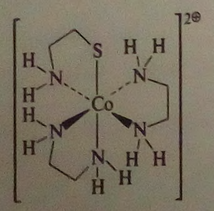


M 271.2 (ion)
Octahedral.
Bis(thiocyanate): [68645-81-8].
Amber coloured cryst. Sol. H_2O.

Kofi Adzamli, I. *et al*, *Inorg. Chem.*, 1979, **18**, 303 (*synth, cryst struct, uv, ir*)

$C_6H_{22}CoN_5S^{2\oplus}$ IC-005478

(2-Aminoethanethiolato-*N,S*)bis(ethylenediamine-*N,N'*)cobalt(*III*)(2+)
[42901-32-6]

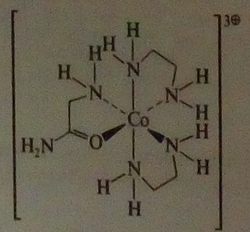


M 255.2 (ion)
Diperchlorate: [64726-53-0].
Black cryst. Stable indefinitely in air; stable for days in dil. aq. acid soln. at 60°. Sol. H_2O, DMF, DMSO, MeOH.

Inorg. Synth., 1982, **21**, 19 (*synth, uv*)

$C_6H_{22}CoN_6O^{3\oplus}$ IC-005479

Bis(ethylenediamine)glycinamidecobalt(*III*)(3+)
(*2-Aminoacetamide*-N^2,O)*bis(1,2-ethanediamine*-N,N')*cobalt*(*3+*), *9CI*
[30931-79-4]



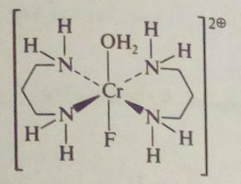
M 253.2 (ion)
Dinitrate, perchlorate: [62319-87-3].
Orange cryst. (dil. aq. $HClO_4$).

[17805-52-6, 62357-85-1]

Buckingham, D.A. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 4539; 1970, **92**, 5571; 1972, **94**, 8246 (*synth, pmr*)

$C_6H_{22}CrFN_4O^{2\oplus}$ IC-005480

Aquafluorobis(1,3-propanediamine-*N,N'*)chromium(*III*)(2+), 11CI, 10CI
[42476-39-1]



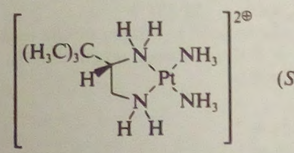
M 237.2 (ion)
trans-Octahedral cation.
Diperchlorate: [19457-69-3].
Red cryst.
Dibromide: [104550-07-4].
Corresp. chloride and iodide also known.

[42476-40-4, 99665-29-9, 104550-06-3]

Solans, X. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2899 (*cryst struct*)

$C_6H_{22}N_4Pt^{2\oplus}$ IC-005481

Diammine(3,3-dimethyl-1,2-butanediamine-*N,N'*)platinum(*II*)(2+), 9CI
Diammine(1,2-diamino-3,3-dimethylbutane)platinum(II)(*2+*)



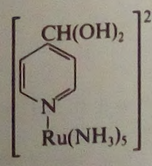
(*S*)-*form*

M 345.3 (ion)
(S)-form
Dichloride: [80145-76-2].
No phys. props. reported.

Hambley, T.W. *et al*, *Aust. J. Chem.*, 1981, **34**, 2505 (*conform, pmr*)
Hawkins, C.J. *et al*, *Inorg. Chem.*, 1982, **21**, 1074 (*synth, pmr, uv*)

$C_6H_{22}N_6O_2Ru^{2\oplus}$ IC-005482

Pentaammine(4-pyridinylmethanediol-*N*)ruthenium(2+)
Pentaammine[*4-(dihydroxymethyl)pyridine*-N]*ruthenium*(II)(*2+*)
[19482-33-8]



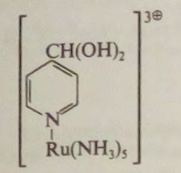
M 311.3 (ion)
Only observed in soln. Formed in aq. soln. by dissolution of Pentaammine(4-pyridinecarboxaldehyde-*N'*)ruthenium(*III*)(2+), IC-005458. Transient higher

concentrations can be achieved by reduction of its ruthenium(*III*) analogue with $[V(OH_2)_6]^{2\oplus}$. In equilibrium with Pentaammine(4-pyridinecarboxaldehyde-*N'*)ruthenium(*III*)(2+), IC-005458 in H_2O with less than 10% in the hydrated form. Sol. H_2O.

Ford, P. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 1187 (*synth, uv, electrochem*)
Zanella, A.W. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 7166 (*synth, uv, dynamic equilibrium*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*electrochem, uv*)

$C_6H_{22}N_6O_2Ru^{3\oplus}$ IC-005483

Pentaammine(4-pyridinylmethanediol-*N*)ruthenium(3+)
Pentaammine[*4-(dihydroxymethyl)pyridine*]*ruthenium*(III)(*3+*), *9CI*
[58580-98-6]

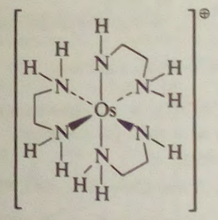


M 311.3 (ion)
Observed in soln. in an equilibrium hydration of Pentaammine(4-pyridinecarboxaldehyde-N^1)ruthenium(3+), IC-005460; the diol is the major species. Sol. H_2O.

Zanella, A.W. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 7166 (*synth, hydration*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*synth, electrochem*)

$C_6H_{22}N_6Os^{\oplus}$ IC-005484

Bis(1,2-ethanediaminato)(1,2-ethanediamine)osmium(*III*)(1+)

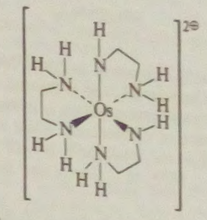


M 368.4 (ion)
Iodide: [15613-67-9].
Synth. from $[Os(en)_3]I_3$ and KNH_2.

Watt, G.W. *et al*, *Inorg. Chem.*, 1966, **5**, 857 (*synth*)

$C_6H_{22}N_6Os^{2\oplus}$ IC-005485

Bis(1,2-ethanediaminato)(1,2-ethanediamine)osmium(*IV*)(2+)
[111614-75-6]

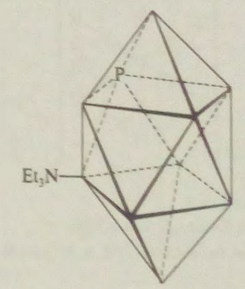


M 368.4 (ion)
Dibromide: [16923-53-8].
Synth. from $(NH_4)_2[OsBr_6]$ with ethylenediamine. Pink cryst. (EtOH aq.).
Diodide: [20623-30-7].
Synth. from bromide with NaI. Pink cryst. (EtOH aq.).

Dwyer, F.P. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 6152 (*synth*)
Lay, P.A. *et al*, *Aust. J. Chem.*, 1987, **40**, 1267 (*cryst struct*)

$C_6H_{23}B_9NP$ IC-005486

2-Phosphadecaborane(8)-6-triethylamine adduct

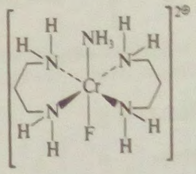


M 237.5
closo-. Colourless cryst. ($CHCl_3$/heptane). Sol. $CHCl_3$. Mp 145-147°.

Little, J.L. *et al*, *Inorg. Chem.*, 1989, **28**, 1087 (*synth, ir, pmr, B-11 nmr, P-31 nmr, ms, cryst struct*)

$C_6H_{23}CrFN_5^{2\oplus}$ IC-005487

Amminefluorobis(1,3-propanediamine-*N,N'*)chromium(*III*)(2+), 11CI, 10CI



M 236.2 (ion)
trans-Octahedral geometry about Cr. Interatomic distances; Cr—F 187.2, Cr—NH_3 208.0 pm.
Diperchlorate: [77462-46-5].
Orange cryst. (H_2O).
Bromide, perchlorate: [77462-45-4].
Orange solid. Sol. H_2O.

Vaughn, J.W., *Inorg. Chem.*, 1981, **20**, 2397 (*cryst struct, synth, uv-vis*)

IC-005488

$C_6H_{23}IrP_2$

Pentahydrobis(trimethylphosphine)iridium, 9CI

Pentahydridobis(trimethylphosphine)iridium(V), *11CI*

[29497-68-5]

$IrH_5(PMe_3)_2$

M 349.4

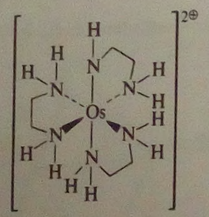
Initially incorrectly formulated as $IrH_3(PMe_3)_2$. Catalyses the exchange between D_2 and aromatics, and also the hydrogenation and isomerisation of alkenes and dehydrogenation of cyclooctane. White air-sensitive cryst. by subl. at r.t. *in vacuo*. V. sol. all org. solvs. Mp 70° dec. Ir ν_{IrH} 1920 cm^{-1}. Slowly dec. in C_6H_6 to liberate H_2.

Barefield, E.K. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 5234 (*synth, nmr, use*)
Klabunde, U. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 9081 (*use*)
Inorg. Synth., 1974, **15**, 34 (*synth, nmr, props*)
Clerici, M.G. *et al*, *J. Organomet. Chem.*, 1975, **84**, 379 (*use*)
Felkin, H. *et al*, *Tetrahedron Lett.*, 1984, **25**, 1279 (*reacts*)

IC-005489

$C_6H_{23}N_6Os^{2\oplus}$

(1,2-Ethanediaminato)bis(1,2-ethanediamine)osmium(*III*)(2+)



M 369.4 (ion)

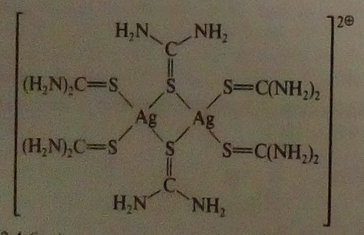
Diiodide: [15613-73-7].
Synth. from $[Os(en)_3]I_3$ and KNH_2.

Watt, G.W. *et al*, *Inorg. Chem.*, 1966, **5**, 857 (*synth*)

IC-005490

$C_6H_{24}Ag_2N_{12}S_6^{2\oplus}$

Bis[μ-(thiourea-*S*:*S*)]tetrakis(thiourea-*S*)disilver(*I*)(2+), 10CI



M 672.4 (ion)

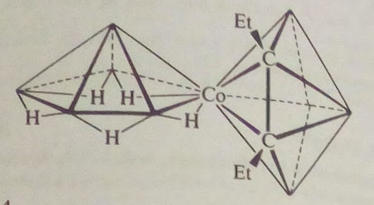
Diperchlorate: [49660-73-3].
Cryst.
▷ Potentially explosive.

Udupa, M.R. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 271 (*synth, cryst struct*)

$C_6H_{24}B_9Co$ IC-005491

[η³-Decahydropentaborato(2−)-*H,H'*][(2,3,4,5,6-η)-2,3-diethyl-1,4,5,6-tetrahydro-2,3-dicarbahexaborato(1−)]cobalt, 11CI

[80583-51-3]



M 252.4

Air-stable orange oil (CH_2Cl_2/hexane by chromatog.). Sol. $CHCl_3$, CH_2Cl_2.

Borodinsky, L. *et al*, *Inorg. Chem.*, 1982, **21**, 1921 (*synth, ir, pmr, B-11 nmr, ms, struct*)

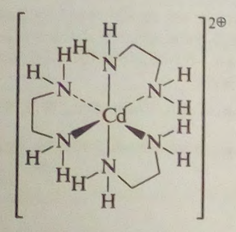
IC-005492

$C_6H_{24}CdN_6^{2\oplus}$

Tris(ethylenediamine)cadmium(2+)

Tris(*1,2-ethanediamine*-N,N')*cadmium*(2+), *9CI*

[18153-92-9]



M 292.7 (ion)

Dichloride: [15613-78-2].
$C_6H_{24}CdCl_2N_6$ M 363.6
Prepd. from $CdCl_2$ + 1,2-ethanediamine. Colourless cryst. (H_2O).

Dihydroxide: [14874-24-9]. *Cadoxen*
$C_6H_{26}CdN_6O_2$ M 326.7
Prepd. from $Cd(OH)_2$ + ethylenediamine. Used in the paper industry as a solv. for cellulose.

[56123-54-7, 92798-55-5]

Schaap, W.B. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 4699 (*formn const*)
Reimers, H., *Papier*, 1962, **16**, 566; *CA*, **63**, 5515a (*synth, use, hydroxide*)
Krishnan, K. *et al*, *Inorg. Chem.*, 1966, **5**, 852 (*synth, raman, ir*)
Fujita, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 930 (*struct, soln*)
Mahadevan, C. *et al*, *Z. Kristallogr.*, 1985, **171**, 173 (*cryst struct, iodide*)
Munakata, M. *et al*, *Inorg. Chem.*, 1986, **25**, 964 (*Cd-113 nmr*)

IC-005493

$C_6H_{24}CdN_{12}O_6^{2\oplus}$

Hexakis(urea-*O*)cadmium(2+)

$[Cd[O{=}C(NH_2)_2]_6]^{2\oplus}$

M 472.7 (ion)
Octahedral cation.

Bis-tetrafluoroborate: [50937-47-8].
White cryst. Mp 147-149°.

Diperchlorate: [38587-21-2].
Solid. Mp 217°. Phase change at 105°.
▷ Potentially explosive.

de Bolster, M.W.G. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 439 (*synth, tetrafluoroborate*)
Karnaukhov, A.S. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 446 (*phase system, synth, powder struct, thermal anal, ir*)
Barbier, J.P. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1976, **95**, 213 (*ir*)

IC-005494

$C_6H_{24}CdN_{12}S_6^{2\oplus}$

Hexakis(thiourea-*S*)cadmium(2+)

[23105-10-4]

$[(H_2N)_2C{=}S]_6Cd^{2\oplus}$

M 569.1 (ion)
Coordination is through the S atom.

Diperchlorate: [51424-75-0].
Prepd. from $Cd(ClO_4)_2$ + thiourea. White cryst. Spar. sol. H_2O. Potentially explosive.

Lane, T.J. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 315 (*formn, const*)
Fedorov, V.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1973, **18**, 1778 (*synth*)

IC-005495

$C_6H_{24}CdO_6^{2\oplus}$

Hexakis(methanol-*O*)cadmium(2+)

$[Cd(MeOH)_6]^{2\oplus}$

M 304.6 (ion)
Octahedral cation. Salts synth. from $[Cd(H_2O)_6]X_2$ and $(MeO)_3CH$.

Bis-tetrafluoroborate: [36051-21-5]. *Cadmium tetrafluoroborate hexamethanol*
White cryst. Mp 86°.

Dinitrate: [36051-27-1]. *Cadmium nitrate hexamethanol*
White cryst. Mp ~25°.

van Ingen Schenau, A.D. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1972, **91**, 88 (*synth, ir*)

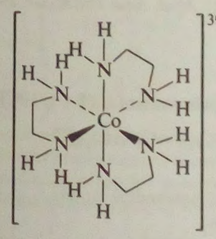
IC-005496

$C_6H_{24}CoN_6^{3\oplus}$

Tris(ethylenediamine)cobalt(*III*)(3+)

Tris(*1,2-ethanediamine*-N,N')*cobalt*(3+), *9CI*

[14878-41-2]



Δ-*form*

M 239.2 (ion)
Used to ppt. many anions. Can be resolved.

Δ-form [16569-46-3]
(−)-*form*

Λ-form [27228-84-8]
(+)-*form*

Trichloride: [26374-64-1].
Orange-red prisms + $1H_2O$; readily loses H_2O in air at r.t.

Tribromide: [35362-43-7].
Orange-red prisms + $1H_2O$.

(±)-*form*

Trichloride: [13408-73-6].
Orange-yellow needles. Sol. H_2O. Dec. >200°.

Tribromide: [13963-67-2].
Golden cryst. Sol. H_2O; sl. sol. EtOH.

Triiodide: [15375-81-2].
Golden cryst. (H_2O). Sol. H_2O; sl. sol. EtOH. Also obt. as hydrate.

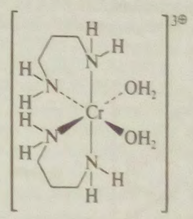
[14883-80-8, 14976-07-9, 15405-85-3, 20468-63-7, 23778-88-3, 29058-84-2, 35270-47-4, 37433-43-5]

Jorgensen, S.M., *J. Prakt. Chem.*, 1889, **39**, 8 (*synth*)
Inorg. Synth., 1946, **2**, 221; 1973, **14**, 58 (*synth, uv-vis*)
Saito, Y. *et al*, *Acta Crystallogr.*, 1955, **8**, 729 (*cryst struct, abs config*)
Nakatsu, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1956, **29**, 428; 1962, **35**, 832 (*synth*)
Raymond, K.N. *et al*, *Inorg. Chem.*, 1968, **7**, 1362 (*synth*)
Iwata, M. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 2562 (*cryst struct, abs config, chloride*)
Witiak, D. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 2694 (*cryst struct, abs config, nitrate*)
Bok, L.D.C. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **389**, 307 (*cryst struct*)
Whuler, A. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 2069; 1980, **36**, 1086 (*cryst struct, synth, iodide monohydrate, (±)*)
Brouty, C. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 2153 (*cryst struct, thiocyanate, (±)-form*)

$C_6H_{24}CrN_4O_2^{3\oplus}$ IC-005497

Diaquabis(1,3-propanediamine-*N,N'*)chromium(*III*)(3+), 11CI, 10CI, 9CI

[38985-24-9]



cis-form

M 236.2 (ion)
Octahedral cation.

cis-form

Trinitrate: Orange plates.

trans-form

Trinitrate: [72919-20-1].
Red-brown needles.

[38985-25-0, 72919-19-8]

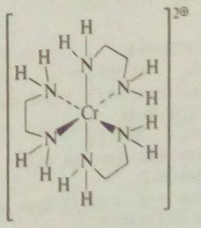
Nakano, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 3563 (*synth, uv-vis, ir*)

IC-005498

$C_6H_{24}CrN_6^{2\oplus}$

Tris(ethylenediamine)chromium(*II*)(2+), 8CI

Tris(*1,2-ethanediamine*-N,N')*chromium*(2+), *11CI, 9CI*



M 232.2 (ion)

Tetragonally distorted octahedral cation. Used in soln. as a reducing agent for organic synth.

Dichloride: [26395-41-5].
$C_6H_{24}Cl_2CrN_6$ M 303.1
Synth. from hydrated Cr(*II*) chloride + ligand in EtOH. Air-sensitive blue cryst. Sol. H_2O and DMF giving solvated $Cr[H_2NCH_2CH_2NH_2]_2^{2\oplus}$. $\mu_{eff} = 4.84\mu_B$ (90-300K).

Dibromide: [26395-42-6].
$C_6H_{24}Br_2CrN_6$ M 392.1
Air-sensitive blue cryst. $\mu_{eff} = 4.75\mu_B$ (90-300K).

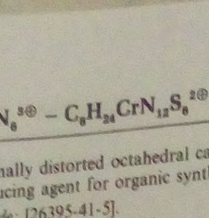
Sulfate: [26395-43-7].
Synth. from ligand and conc. aq. $CrSO_4.5H_2O$. Air-sensitive light blue cryst. $\mu_{eff} = 4.87\mu_B$ (90-300K).

Dicyclopentadienide: [104818-09-9].
$C_{16}H_{34}CrN_6$ M 362.4
Synth. by reaction of chromocene with $H_2NCH_2CH_2NH_2$. Air-sensitive grey-blue powder. Insol. C_6H_6, hexane, Et_2O; sol. (with dec.) H_2O, EtOH. $\mu_{eff} = 4.80\mu_B$.

Pecsok, R.L. *et al*, *Acta Chem. Scand.*, 1957, **11**, 1419 (*stability const*)
Larkworthy, L.F. *et al*, *J. Chem. Soc. A*, 1969, 1339 (*synth, props*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 142 (*use*)
Ho, T.L., *Synthesis*, 1979, 1 (*use*)
Kalousova, J. *et al*, *Collect. Czech. Chem. Commun.*, 1986, **51**, 314.

$C_6H_{24}CrN_6^{3\oplus}$ IC-005499

Tris(ethylenediamine)chromium(*III*)(3+), 8CI
*Tris(1,2-ethanediamine-*N,N′*)chromium(3+), 11CI, 10CI, 9CI*
[15276-13-8]



Δ-form

M 232.2 (ion)
Octahedral. Salts sl. light sensitive. Dec. slowly aq. soln.; many salts known.

Δ-form [51002-41-6]
(−)-form
Tribromide: [39023-33-1].
Triiodide: [20594-26-7].
Trithiocyanate: Cryst. $[\alpha]_D$ −87° (aq. soln.).

Λ-form [41509-53-9]
(+)-form
Trichloride: [30983-64-3].
Cryst. + $2H_2O$. $[\alpha]_D$ +108°.
Tribromide: Cryst. + 0.6 H_2O.

(±)-form
Trichloride: [14023-00-8].
$C_6H_{24}Cl_3CrN_6$ M 338.6
Orange-yellow cryst. (H_2O). V. sol. H_2O.
Tribromide: [14267-09-5].
$C_6H_{24}Br_3CrN_6$ M 472.0
Orange-yellow cryst. Spar. sol. H_2O.
Triiodide: [14049-58-2].
Orange-yellow cryst. + $1H_2O$. Spar. sol. H_2O.
Trithiocyanate: [14176-00-2].
Orange-yellow cryst. (H_2O). Spar. sol. H_2O.
Sulfate (2:3): [13408-71-4].
Orange-yellow cryst. V. sol. H_2O.
[31125-86-7, 33702-30-6]

Brauer, G., *Handbook of Preparative Inorganic Chemistry*, 2nd Edn., 1965-71, Academic Press, N.Y., 1965, **2**, 1354 (*synth*)
Raymond, K.N. *et al*, *Inorg. Chem.*, 1968, **7**, 1362, 2333 (*cryst struct*)
Garner, C.S. *et al*, *Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Brouty, C. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 2877, 3453 (*cryst struct, abs config*)
Whuler, A. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 793 (*cryst struct, Λ-form, chloride*)
Spinat, P. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2914 (*cryst struct, Δ-form, bromide*)
Inorg. Synth., 1979, **19**, 123 (*synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 789 (*rev*)

$C_6H_{24}CrN_{12}O_6^{3\oplus}$ IC-005500

Hexakis(urea-*O*)chromium(*III*)(3+), 11CI, 10CI, 9CI
Hexaureachromium(III)(3+)
[15276-06-9]

$$Cr[O{=}C(NH_2)_2]_6^{3\oplus}\ (O_h)$$

M 412.3 (ion)
Cr—O 196.0 to 198.2 pm. Starting material. Many salts.
Trichloride: [14023-01-9]. *Chromium*(III) *chloride hexakis-urea*
$C_6H_{24}Cl_3CrN_{12}O_6$ M 518.6
Synth. from green $[CrCl_2(OH_2)_4]Cl.2H_2O$ and urea in v. dil. HCl. Green needles + $3H_2O$ (min. H_2O). Sol. H_2O; insol. EtOH.
▷ GB5475000.
Triperchlorate: [15221-22-4].
[27459-64-9]

Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1503 (*synth*)
Flint, C.D. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1979, 1159 (*uv, photochem*)
Yamada, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 3596 (*electrochem*)
Niven, M.L. *et al*, *Cryst. Struct. Commun.*, 1980, **9**, 1133 (*cryst struct*)
Rau, V.G. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1982, **267**, 1371 (*cryst struct*)
Figgis, B.N. *et al*, *Aust. J. Chem.*, 1984, **37**, 265 (*cryst struct*)
Bondar, V.I. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1984, **279**, 373 (*cryst struct*)

$C_6H_{24}CrN_{12}S_6^{2\oplus}$ IC-005501

Hexakis(thiourea-*S*)chromium(*II*)(2+), 10CI

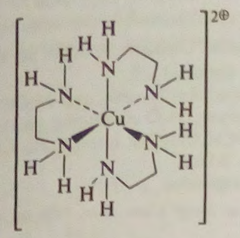
$$[Cr[S{=}C(NH_2)_2]_6]^{2\oplus}$$

M 508.7 (ion)
Presumably distorted octahedral struct.
Diiodide: [74624-97-8].
$C_6H_{24}CrI_2N_{12}S_6$ M 762.5
Yellow-green solid. $\mu_{eff} = 4.77\mu_B$ (temp. independent).

Larkworthy, L.F. *et al*, *Inorg. Chim. Acta*, 1980, **40**, 217 (*synth, uv, ir*)

$C_6H_{24}CuN_6^{2\oplus}$ IC-005502

Tris(ethylenediamine)copper(*II*)(2+)
*Tris(1,2-ethanediamine-*N,N′*)copper(2+), 9CI*
[21556-23-0]

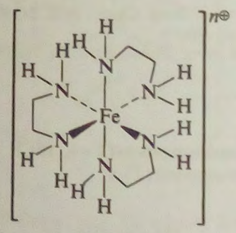


M 243.8 (ion)
Octahedral.
Sulfate: [15613-88-4].
Purple hexagonal cryst.
Diperchlorate: [37662-44-5].
Dichloride:
$C_6H_{24}Cl_2CuN_6$ M 314.7

Gorden, G. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 3567 (*synth, uv, ir*)
Cola, M. *et al*, *Atti Accad. Sci. Torino, Cl. Sci. Fis., Mat. Nat.*, 1962, **96**, 381 (*synth*)
Cullen, D.L. *et al*, *Inorg. Chem.*, 1970, **9**, 1858 (*synth, cryst struct*)
Escard, J. *et al*, *Bull. Groupe Fr. Argiles*, 1973, **25**, 181 (*pe*)
Mitra, S.N. *et al*, *Indian J. Phys.*, 1973, **47**, 79 (*magnetism*)
Bertini, I. *et al*, *Inorg. Chim. Acta*, 1974, **11**, L17 (*esr*)

$C_6H_{24}FeN_6^{2\oplus}$ IC-005503

Tris(ethylenediamine)iron(*II*)(2+), 8CI
*Tris(1,2-ethanediamine-*N,N′*)iron(2+), 11CI, 9CI. Tris(1,2-diaminoethane)iron*(II)(2+)
[14972-42-0]



$n = 2$

M 236.1 (ion)
Octahedral cation. Synth. from air-free Fe(*II*) salts and anhydrous ethylenediamine. Precursor for macrocyclic complexes. Large cation for precipitation of large anions. Redox active. Has not been resolved.
Dichloride:
$C_6H_{24}Cl_2FeN_6$ M 307.0
White solid; oxidises rapidly in air → brown. $\mu_{eff} = 5.45\mu_B$.
Diperchlorate: Light brown cryst. Sol. Me_2CO.
Tetracarbonylferrate(2−): [107766-77-8].
Synth. from $Fe_4(CO)_8(Py)_4$ + ethylenediamine.

Breuil, M.R.E., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1933, **196**, 2009 (*synth*)
Fowles, G.W.A. *et al*, *J. Chem. Soc.*, 1958, 136 (*synth*)
Sadasivan, N. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 5468 (*synth*)
Paoletti, P., *Pure Appl. Chem.*, 1984, **56**, 491 (*rev*)

$C_6H_{24}FeN_6^{3\oplus}$ IC-005504

Tris(ethylenediamine)iron(*III*)(3+)
*Tris(1,2-ethanediamine-*N,N′*)iron*(III)(3+), *9CI. Tris(1,2-diaminoethane)iron*(III)(3+)
As Tris(ethylenediamine)iron(*II*)(2+), IC-005503 with

$n = 3$

M 236.1 (ion)
Low spin octahedral cation. Flame retardant for cotton.
Trichloride: [20683-83-4].
$C_6H_{24}Cl_3FeN_6$ M 342.5
Synth. from $FeCl_3$ + ethylenediamine in EtOH. Flesh-coloured solid, stable in dry air. Low spin, $\mu_{eff} = 2.45\mu_B$ (r.t.), $2.17\mu_B$ (80K).

Renovitch, G.A. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 3585 (*synth, ir, mössbauer*)
Reiff, W.M., *Chem. Phys. Lett.*, 1971, **8**, 297 (*mössbauer*)
Garg, A.N. *et al*, *Indian J. Chem.*, 1974, **12**, 996 (*mössbauer*)

$C_6H_{24}FeN_{12}O_6^{3\oplus}$ IC-005505

Hexakis(urea-*O*)iron(3+), 9CI, 8CI
[34943-83-4]

$$[Fe[O{=}C(NH_2)_2]_6]^{3\oplus}$$

M 416.1 (ion)
Presumed octahedral cation.
Trichloride: [15613-85-1]. *Iron*(III) *chloride hexakis-urea*
$C_6H_{24}Cl_3FeN_{12}O_6$ M 522.5
Cryst. Sl. sol. H_2O. $\mu_{eff} = 5.56\mu_B$.
Tribromide: [70305-00-9]. *Iron*(III) *bromide hexakis-urea*
$C_6H_{24}Br_3FeN_{12}O_6$ M 655.8
Cryst. Sl. sol. H_2O. $\mu_{eff} = 6.01\mu_B$.
Trinitrate: [15613-89-5]. *Iron*(III) *nitrate hexakis-urea*
Pale green (colourless) cryst. Sl. sol. H_2O.
Triperchlorate: [21338-24-9]. *Iron*(III) *perchlorate hexakis-urea*
V. pale green cryst. Sl. sol H_2O. Mp 202°. $\mu_{eff} = 5.76\mu_B$.

Hok, S. *et al*, *Acta Chem. Scand.*, 1968, **22**, 1091 (*uv-vis*)
Cotton, S.A. *et al*, *J. Chem. Soc. A*, 1971, 1690 (*synth, ir, raman, esr*)
Fatta, A.M. *et al*, *Inorg. Chem.*, 1972, **11**, 88 (*uv-vis*)
Durski, Z. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1972, **46**, 1945 (*struct*)
Calogero, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 646 (*mössbauer, magnetism*)
Russo, U. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **41**, 25 (*magnetism, mössbauer, ir*)
Galeazzi, G. *et al*, *Transition Met. Chem.*, 1981, **6**, 325 (*mössbauer*)
Lupin, M.S. *et al*, *Thermochim. Acta*, 1984, **73**, 79 (*thermal anal*)

$C_6H_{24}IrN_{12}S_6^{3\oplus}$ IC-005506

Hexakis(thiourea-*S*)iridium(*III*)(3+)
Hexathioureairidium(III)(3+), *8CI*

$$Ir[S{=}C(NH_2)_2]_6^{3\oplus}$$

M 648.9 (ion)
Trichloride: [23623-86-1].
$C_6H_{24}Cl_3IrN_{12}S_6$ M 755.3
Green cryst. Sol. H_2O.

Grinberg, A.A. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1969, **14**, 309 (*synth*)

IC-005507

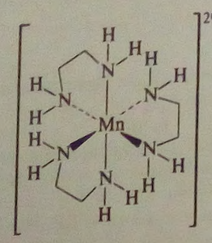
$C_6H_{24}MnN_6^{2\oplus}$

Tris(ethylenediamine)manganese(*II*)(2+)

Tris(1,2-ethanediamine-N,N′)manganese(2+), 1ICl

Tris[1,2-diaminoethane]manganese(II)(2+)

[23281-19-8]



M 235.2 (ion)

Octahedral cation. Catalyses dec. of H_2O_2 and accelerates photopolym. of vinyl monomers in the presence of CCl_4. Air-sensitive; aq. solns. are oxidised. ΔH_f° −434.3 kJ mol^{-1}.

Bis-tetrafluoroborate: Synth. from $Mn(BF_4)_2.6H_2O$ and ethylenediamine hydrate in EtOH. White cryst; turns brown in air. Insol. EtOH, Et_2O.

Diperchlorate: [52689-68-6].

▷ Potentially explosive.

Thiosulfate: [19955-62-5].

$C_6H_{24}MnN_6O_3S_2$ M 347.3

Synth. from 0.5*M* aq. solns. of $MnSO_4$,$K_2S_2O_3$ and calculated amount of 20% ethylenediamine. Pale brown cryst; darkens in air.

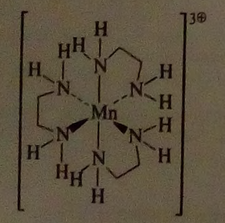
Spacu, G. *et al*, *Z. Anorg. Allg. Chem.*, 1935, **223**, 185 (*synth*)
Joørgensen, C.K., *Acta Chem. Scand.*, 1957, **11**, 53 (*vis*)
Chiswell, B. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 707 (*synth*)
Mui, K.K., *Can. J. Chem.*, 1974, **52**, 1821 (*props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 37 (*rev, bibl*)
Xie, Z. *et al*, *CA*, 1984, **100**, 131827f.

IC-005508

$C_6H_{24}MnN_6^{3\oplus}$

Tris(ethylenediamine)manganese(*III*)(3+), 8Cl

Tris(1,2-diaminoethane)manganese(3+)



M 235.2 (ion)

Octahedral cation.

Triperchlorate: Synth. from solid $[Mn(urea)_6](ClO_4)_3$ + ethylenediamine in MeCN. Air-sensitive green powder (EtOH). $\mu_{eff} = 4.85\mu_B$.

▷ Potentially explosive.

Summers, J.C., *Diss. Abstr. Int., B*, 1969, **30**, 109 (*synth, magnetism, esr, uv, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 42 (*rev, bibl*)

IC-005509

$C_6H_{24}MnN_{12}O_6^{2\oplus}$

Hexakis(urea-*O*)manganese(2+), 1ICl

Hexa(urea)manganese(2+)

$[Mn[O{=}C(NH_2)_2]_6]^{2\oplus}$

M 415.2 (ion)

Octahedral cation. Unstable in dilute aq. soln.

Diperchlorate: [38845-37-3].

Prepared from $MnCl_2$, urea, and $NaClO_4$ in EtOH. Colourless cryst. (H_2O containing urea). Sol. H_2O, EtOAc, $HOCH_2CH_2OH$; insol. C_6H_6, $CHCl_3$, Et_2O. Mp 190°. $\mu_{eff} = 5.86\mu_B$.

▷ Potentially explosive.

Barbier, J.P. *et al*, *Inorg. Chim. Acta*, 1974, **10**, 93 (*synth, ir, esr, magnetism*)
Kaglin, E. *et al*, *Z. Naturforsch., A*, 1978, **33**, 377 (*synth, uv-vis*)
Goryunov, Yu.A., *CA*, 1982, **97**, 65413 (*dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 139 (*rev, bibl*)

IC-005510

$C_6H_{24}MnN_{12}O_6^{3\oplus}$

Hexakis(urea-*O*)manganese(3+), 1ICl

$[Mn[O{=}C(NH_2)_2]_6]^{3\oplus}$

M 415.2 (ion)

Contains 6 equivalent Mn—O bonds. Uv consistent with a dynamic Jahn-Teller effect.

Triperchlorate: [82823-06-1]. *Manganese*(III) *perchlorate hexakis(urea)*

$C_6H_{24}Cl_3MnN_{12}O_{18}$ M 713.6

Synth. from a hot soln. of $Mn(OAc)_2$ in AcOH, $KMnO_4$ and urea in $HClO_4$. Dark purple cryst. ($HClO_4$ sat. with urea), unstable in air, dec. by H_2O. Insol. EtOH, Et_2O. $\mu_{eff} = 5.02\mu_B$, high spin d^4.

▷ Potentially explosive.

Aghabozorg, H. *et al*, *Inorg. Chem.*, 1982, **21**, 3903 (*synth, magnetism, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 140 (*rev, bibl*)

IC-005511

$C_6H_{24}MnO_6^{2\oplus}$

Hexakismethanolmanganese(2+), 1ICl

Hexamethanolmanganese(2+)

[21563-12-2]

$[Mn(MeOH)_6]^{2\oplus}$

M 247.1 (ion)

Prepd. from MnX_2 hydrates and trimethyl orthoformate (X = BF_4, ClO_4, NO_3). MeOH ligands easily replaced by H_2O.

Diperchlorate: [36051-14-6]. *Manganese*(II) *perchlorate hexamethanol*

Colourless powder.

▷ Potentially explosive.

Bis-tetrafluoroborate: [36051-17-9].

Colourless powder.

Dinitrate: [36051-23-7].

Colourless powder.

Levanonon, H. *et al*, *J. Chem. Phys.*, 1968, **49**, 2031 (*esr, nmr*)
Wells, C.F., *J. Chem. Soc. A*, 1968, 1626; 1971, 430 (*props*)
Dickert, F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1972, 106 (*stability const*)
Van Ingen Schenau, A.D. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1972, **91**, 88 (*synth*)
de Bolster, M.W.G. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 2106 (*synth, ir*)

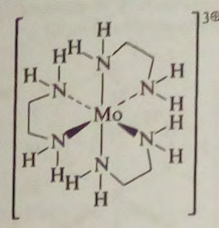
Tiezzi, E. *et al*, *Org. Magn. Reson.*, 1975, **7**, 602 (*pmr, cmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 25 (*rev, bibl*)

IC-005512

$C_6H_{24}MoN_6^{3\oplus}$

Tris(ethylenediamine)molybdenum(*III*)(3+)

Tris(1,2-ethanediamine-N,N′)molybdenum(3+), 9Cl



M 276.2 (ion)

Trithiocyanate: [53480-14-1].

Synth. by treatment of $(NH_4)_3[Mo(NCS)_6]$ with ethylenediamine. Yellow cryst. $\mu_{eff} = 3.65\mu_B$ (300K).

Ghosh, S.P. *et al*, *J. Less-Common Met.*, 1974, **36**, 223 (*deriv*)
Ghosh, S.P. *et al*, *Proc. First Int. Conf. Chemistry and Uses of Molybdenum*, Ed., P.C.H Mitchell, Climax Molybdenum Co., Ann Arbor, MI, 1974, 119 (*deriv*)

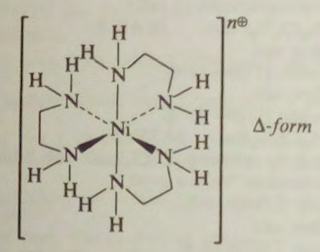
IC-005513

$C_6H_{24}N_6Ni^{2\oplus}$

Tris(ethylenediamine)nickel(*II*)(2+), 8Cl

Tris(1,2-ethanediamine-N,N′)nickel(II)(2+), *9Cl*

[15390-99-5]



n = 2

M 238.9 (ion)

Extremely well-studied ion. Kinetically labile. Reacts with Me_2CO and carbonyl compds. to form polydentate amine-imine ligands.

Δ-form

(−)-*form*

Dinitrate: [73460-29-4].

Synth. from slow evap. of aq. $Ni(NO_3)_2$ soln. and excess ethylenediamine; spontaneously resolves. Dark purple cryst. Extensively H-bonded. Interatomic distances: Ni—N 213, N—C 147.6 pm; angles: NNiN 81.9°, NiNC 108.1°.

Λ-form

Dinitrate: [55524-15-7].

Violet cryst. Dec. at 270° on slow heating.

▷ Dec. explosively if heated rapidly.

(±)-*form*

Dichloride: [13408-70-3].

Blue cryst.

Dibromide: [14896-63-0].

Violet cryst. Sol. H_2O; insol. Me_2CO.

Dinitrate: [14405-81-3].

$C_6H_{24}N_8NiO_6$ M 362.9

Blue-violet cryst. (H_2O). Fairly sol. H_2O.

Diperchlorate: [14095-89-7].

Violet solid. Paramagnetic; $\mu_{eff} = 3.21\mu_B$.

Dichloride, dihydrate: [33908-61-1].

Prismatic, violet cryst. Sol. H_2O.

Diperchlorate, dihydrate: [15747-97-4].

Synth. from $[Ni(en)_3]Cl_2$ and $NaClO_4$ in aq. soln. Purple cryst. Paramagnetic; $\mu_{eff} = 3.21\mu_B$.

Sulfate: [15304-51-5].

$C_6H_{24}N_6NiO_6S$ M 335.0

Needles (hot H_2O). Insol. EtOH; sl. sol. cold H_2O; sol. hot H_2O. Paramagnetic; $\mu_{eff} = 3.16\mu_B$.

Thiosulfate: [20714-34-5].

$C_6H_{24}N_6NiO_3S_2$ M 351.1

Purple cryst. (ice cold Me_2CO or MeOH). Paramagnetic; $\mu_{eff} = 3.09\mu_B$.

[28560-21-6, 28560-22-7]

Werner, A. *et al*, *Z. Anorg. Allg. Chem.*, 1899, **21**, 201 (*synth, derivs*)
Swink, L.N. *et al*, *Acta Crystallogr.*, 1960, **13**, 639 (*cryst struct, nitrate*)
Inorg. Synth., 1960, **6**, 200; 1973, **14**, 57 (*synth, derivs, props*)
Farago, M.E. *et al*, *J. Chem. Soc. A*, 1967, 820 (*synth, perchlorate, magnetism, ir, vis*)
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1968, **IC**, 146 (*many derivs, synth, props*)
Ho, F.F.L. *et al*, *Anal. Chem.*, 1970, **42**, 600 (*conformn, pmr*)
Gabelica, Z., *Spectrochim. Acta, Part A*, 1976, **32**, 327 (*raman, ir, thiosulfate*)
Hawkins, C.J. *et al*, *Acta Chem. Scand., Ser. A*, 1978, **32**, 815 (*conformn, pmr*)
Korp, J.D. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 560 (*synth, cryst struct, abs config, nitrate*)
Lusty, J.R., *J. Coord. Chem.*, 1980, **10**, 243 (*thiosulfate, synth, ir, uv-vis, magnetism*)
El-Sayed, A.B. *et al*, *Chem. Scr.*, 1985, **25**, 318 (*conform, ir, sulfate*)
Compr. Coord. Chem., 1987, **5**, 71, 95, 106, 226; **6**, 163 (*rev, bibl, reactions*)

IC-005514

$C_6H_{24}N_6Ni^{3\oplus}$

Tris(ethylenediamine)nickel(*III*)(3+)

Tris(ethanediamine-N,N′)nickel(III)(3+), *9Cl*

[38467-97-9]

As Tris(ethylenediamine)nickel(*II*)(2+), IC-005513 with

n = 3

M 238.9 (ion)

Formed from reaction of Tris(ethylenediamine)nickel(*II*)(2+), IC-005513 and OH radicals. Unstable.

Lati, J. *et al*, *Inorg. Chem.*, 1972, **11**, 2397.

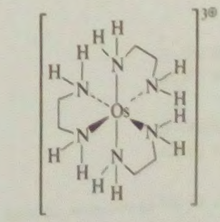
IC-005515

$C_6H_{24}N_6Os^{3\oplus}$

Tris(ethylenediamine)osmium(*III*)(3+)

Tris(1,2-ethanediamine-N,N′)osmium(3+), 1ICl

[46138-85-6]



M 370.4 (ion)

Tris-trifluoromethanesulfonate salt: [111575-90-7].

Synth. from the bromide salt in 6*M* CF_3SO_3H. Colourless cryst. + $1H_2O$.

Lay, P.A. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 6161 (*electrochem*)
Lay, P.A. *et al*, *Aust. J. Chem.*, 1987, **40**, 1267 (*cryst struct, synth*)

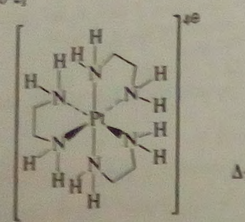
IC-005516

$C_6H_{24}N_6Pt^{4\oplus}$

Tris(ethylenediamine)platinum(*IV*)(4+), 8Cl

Tris(1,2-ethanediamine-N,N')platinum(IV)(*4+*), *9Cl*

[18536-10-2]



Δ-form

M 375.3 (ion)
Chiral ion; can be resolved. Kinetically stable but reacts by photolysis. Ligand reactions known.

(Δ,Δ)-form

(±)-form

Chloride: [12079-33-3].
White cryst. (conc aq. HCl). Sol. H_2O.

Perchlorate: [63057-35-2].
White solid.

[16970-76-6, 17185-78-3, 41673-41-0]

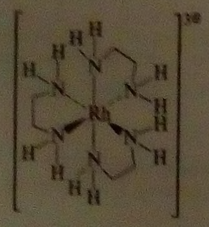
Gmelin Handbook Inorg. Chem., Syst. No. 68, 1957, **D**, 471 (*rev, bibl*)
Inorg. Synth., 1966, **8**, 239 (*synth*)
Liu, C.F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 412 (*optical rotation*)
Appleton, T.G. *et al*, *Inorg. Chem.*, 1970, **9**, 1299 (*pmr*)
James, D.W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 319 (*ir, raman*)
Pesek, J.J. *et al*, *J. Magn. Reson.*, 1977, **25**, 519 (*Pt-195 nmr*)
Harris, R.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1015 (*solid state Pt-195 nmr*)

$C_6H_{24}N_6Rh^{3\oplus}$

IC-005517

Tris(ethylenediamine)rhodium(*III*)(3+)

Tris(1,2-ethanediamine-N,N')rhodium(III)(*3+*), *9Cl*



M 283.2 (ion)

(+)-form

Trichloride: [30983-68-7].
White cryst. + $3H_2O$.

(−)-form

Trichloride: [31125-87-8].
White cryst. + $3H_2O$.

[15307-31-0]

Inorg. Synth., 1970, **12**, 269 (*synth, resoln, cd, prop*)

Addison, A.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 709 (*synth*)
Whuler, P.A. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 2238 (*cryst struct*)

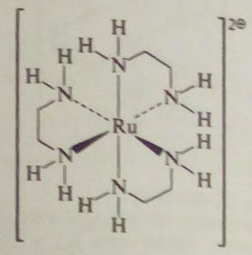
$C_6H_{24}N_6Ru^{2\oplus}$

IC-005518

Tris(ethylenediamine)ruthenium(*II*)(2+), 8Cl

Tris(1,2-ethanediamine-N,N')ruthenium(II)(*2+*), *9Cl*.
Tris(1,2-diaminoethane)ruthenium(II)

[21393-86-2]



M 281.3 (ion)
Pseudooctahedral. The (−) form has a D config.; Ru—N 213.2 pm. Prepd. by reducing '$RuCl_3.xH_2O$' in H_2O with Zn dust in the presence of ethylenediamine. A useful one-electron reducing agent. Sol. H_2O.

(±)-form

Tetrachlorozincate(II) *salt:* [23726-39-8].
$C_6H_{24}Cl_4N_6RuZn$ M 488.5
Yellow salt.

Tetrachloroplatinate(II) *salt:*
$C_6H_{24}Cl_4N_6PtRu$ M 618.2
Yellow salt.

Dibromide: [15699-12-4].
Yellow salt.

Dichloride: [31894-75-4].
$C_6H_{24}Cl_2N_6Ru$ M 352.2
Prepd. by reducing $[ZnCl_4]$-salt with lithium anthranilate. Yellow cryst.

Diiodide: [15699-11-3].
Yellow salt.

Dinitrate: [75458-64-9].
Yellow salt. Other similar salts may be prepd.

Lever, F.M. *et al*, *Platinum Met. Rev.*, 1964, **8**, 106 (*synth*)
Allen, A.D. *et al*, *Can. J. Chem.*, 1965, **43**, 888 (*synth, ir*)
Schmidtke, H.-H. *et al*, *Helv. Chim. Acta*, 1966, **49**, 2039 (*uv*)
Meyer, T.J. *et al*, *Inorg. Chem.*, 1968, **7**, 2369 (*oxidation*)
Elsbernd, H. *et al*, *Inorg. Chem.*, 1969, **8**, 893 (*uv, ord, cd*)
Beattie, J.K. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 1946 (*pmr*)
Pladziewicz, J.R. *et al*, *Inorg. Chem.*, 1973, **12**, 639 (*uv*)
Adegite, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 630 (*oxidation*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1978, **17**, 1747 (*photochem*)
Inorg. Synth., 1979, **19**, 117 (*synth*)
Bernal, I. *et al*, *Inorg. Chem.*, 1981, **20**, 295 (*abs config*)
Smolenaers, P.J. *et al*, *Inorg. Chem.*, 1981, **20**, 2202 (*cryst struct*)

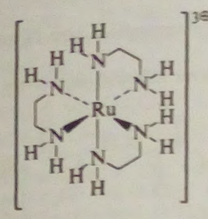
$C_6H_{24}N_6Ru^{3\oplus}$

IC-005519

Tris(ethylenediamine)ruthenium(3+)

Tris(ethylenediamine)ruthenium(III). *Tris(1,2-diaminoethane-N,N')ruthenium*(*3+*), *9Cl*

[21393-87-3]



M 281.3 (ion)
Approx. octahedral with Ru—N 211 pm. Prepd. by the oxidation of Tris(ethylenediamine)ruthenium(*II*)(2+), IC-005518 with I_2 or HNO_3. Useful reagent for electron-transfer reactions. Solns. are oxygen-sensitive, the cation being oxidised to (Ethanediimine-*N,N'*) bis(ethylenediamine-*N,N'*)ruthenium(*II*)(2+), IC-005461. Sol. H_2O.

Trichloride: [31091-62-0].
$C_6H_{24}Cl_3N_6Ru$ M 387.7
Colourless cryst.

Tribromide: [21958-96-3].
$C_6H_{24}Br_3N_6Ru$ M 521.0
Yellow-orange cryst. $\mu_{eff} = 2.13\mu_B$.

Triiodide: [21958-97-4].
$C_6H_{24}I_3N_6Ru$ M 662.0
Dark purple cryst. $\mu_{eff} = 2.24\mu_B$.

[23422-89-1, 23726-40-1]

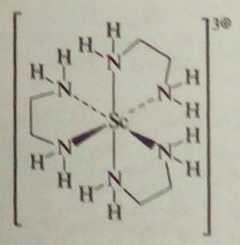
Meyer, T.J. *et al*, *Inorg. Chem.*, 1968, **7**, 2369 (*synth, electrochem, deuteration*)
Elsbernd, H. *et al*, *Inorg. Chem.*, 1968, **7**, 2468; 1969, **8**, 893 (*uv, ord, cd, resol*)
Watt, G.W. *et al*, *Can. J. Chem.*, 1969, **47**, 359 (*synth*)
Peresie, H.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 1674 (*cryst struct*)
Lane, B.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 1618 (*oxidation by O_2*)
Stanko, J.A. *et al*, *Inorg. Chem.*, 1973, **12**, 634 (*esr*)
Lavallee, C. *et al*, *Inorg. Chem.*, 1978, **17**, 2217 (*reduction*)
Inorg. Synth., 1979, **19**, 117 (*synth*)
Iadevia, R. *et al*, *Inorg. Chim. Acta*, 1981, **53**, L143 (*reduction*)
Sisley, M.J. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 225 (*reduction*)

$C_6H_{24}N_6Sc^{3\oplus}$

IC-005520

Tris(ethylenediamine)scandium(*III*)(3+)

Tris(1,2-ethanediamine-N,N')scandium(III)(*3+*), *9Cl*



M 225.2 (ion)

Trichloride: [41592-72-7].
$C_6H_{24}Cl_3N_6Sc$ M 331.6
White cryst. Sl. sol. MeCN; sol. H_2O with dec. Loses 1 ethylenediamine on heating *in vacuo*.

Tomanaev, I.V. *et al*, *Zh. Neorg. Khim.*, 1962, **7**, 2022; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 1045 (*synth*)
Wagner, M.R. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 869 (*synth, ir*)

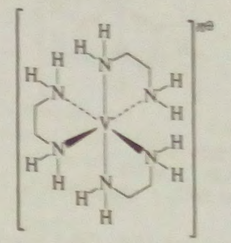
$C_6H_{24}N_6V^{2\oplus}$

IC-005521

Tris(ethylenediamine)vanadium(*II*)(2+), 8Cl

Tris(1,2-ethanediamine-N,N')vanadium(II)(*2+*). *11Cl*.
Tris(1,2-diaminoethane)vanadium(II)(*2+*)

[100481-65-0]



n = 2

M 231.2 (ion)
Octahedral.

Dichloride: [23390-22-9].
$C_6H_{24}Cl_2N_6V$ M 302.1
Synth. by adding ethylenediamine to $VCl_2.6H_2O$ in EtOH. Green, hygroscopic solid. Paramagnetic, μ_{eff} = $3.84\mu_B$ (θ 0K).

Diiodide: [23440-34-8].
Synth. as for the chloride. Green, air-sensitive solid.

Khamer, M. *et al*, *Aust. J. Chem.*, 1974, **27**, 41 (*synth, ir, uv-vis, magnetism*)

$C_6H_{24}N_6V^{3\oplus}$

IC-005522

Tris(ethylenediamine)vanadium(*III*)(3+), 8Cl

Tris(1,2-ethanediamine-N,N')vanadium(III)(*3+*). *Tris(1,2-diaminoethane)vanadium*(III)

As Tris(ethylenediamine)vanadium(*II*)(2+), IC-005521 with

n = 3

M 231.2 (ion)
Octahedral.

Trichloride: [14874-14-7].
$C_6H_{24}Cl_3N_6V$ M 337.5
Synth. by reaction of VCl_3 with pure ethylenediamine. Red-brown solid (ethylenediamine). Paramagnetic, μ_{eff} = $2.92\mu_B$ (300K), $2.83\mu_B$ (78K).

Clark, R.J.H. *et al*, *J. Chem. Soc. A*, 1967, 409 (*synth, uv-vis*)
Machin, D.J. *et al*, *J. Chem. Soc. A*, 1967, 1498 (*magnetism*)
Rupp, H.A., *Z. Anorg. Allg. Chem.*, 1970, **377**, 105 (*synth*)

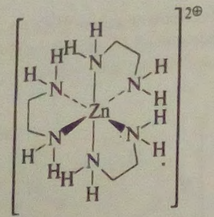
IC-005523

$C_6H_{24}N_6Zn^{2\oplus}$

Tris(ethylenediamine)zinc(2+)

Tris(1,2-ethanediamine-N,N')zinc(2+), 9CI

[16787-16-9]



M 245.6 (ion)

Dichloride: [15613-79-3].
$C_6H_{24}Cl_2N_6Zn$ M 316.5
Prepd. from $ZnCl_2$ + ethylenediamine. Cryst. + $2H_2O$ (H_2O).

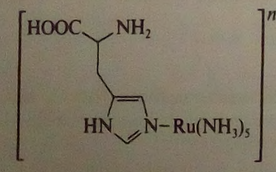
Krishnan, K. *et al, Inorg. Chem.*, 1966, **5**, 852 (*synth, ir, raman*)
Palmer, R.A. *et al, Chem. Phys. Lett.*, 1975, **31**, 492 (*cd, abs config*)
Shevchenko, Yu.N. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1977, **22**, 2872 (*synth*)
Fujita, T. *et al, Bull. Chem. Soc. Jpn.*, 1979, **52**, 3539 (*struct, soln*)
Muralikrishna, C. *et al, Acta Crystallogr., Sect. C*, 1983, **39**, 1630 (*cryst struct, chloride*)

IC-005524

$C_6H_{24}N_8O_2Ru^{2\oplus}$

Pentaammine(histidine)ruthenium(*II*)(2+)

[81845-34-3]



$n = 2$

M 341.3 (ion)

The histidine ligand is bound through N(3). Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with histidine or by Zn/Hg reduction of Pentaammine(DL-histidine-N^3)ruthenium(*III*)(3+), IC-005525.

Diperchlorate: Yellow salt.

Sundberg, R.J. *et al, Bioinorg. Chem.*, 1973, **3**, 39 (*synth, uv, pmr, electrochem*)
Tweedle, M.F. *et al, Inorg. Chem.*, 1982, **21**, 3361 (*isomerization, reaction, electrochem*)

IC-005525

$C_6H_{24}N_8O_2Ru^{3\oplus}$

Pentaammine(histidine)ruthenium(*III*)(3+)

[50726-40-4]

As Pentaammine(histidine)ruthenium(*III*)(2+), IC-005524 with

$n = 3$

M 341.3 (ion)

Trichloride: [50726-52-8].
Synth. from Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 + histidine, followed by aerial oxidation. Orange cryst. pK_a 8.7 (N1); pK_a 7.2 (side chain N).

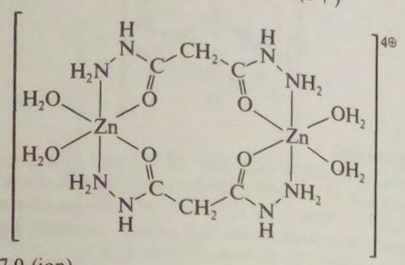
Sundberg, R.J. *et al, Bioinorg. Chem.*, 1973, **3**, 39 (*synth, uv, pK_a*)

IC-005526

$C_6H_{24}N_8O_8Zn_2^{4\oplus}$

Tetraaquabis[μ-(propanedioic acid dihydrazide)]dizinc(4+)

Tetraaquabis[malonic dihydrazide]dizinc(4+)



M 467.0 (ion)

Dinuclear tetracation, containing octahedral Zn in solid state.

Tetranitrate: [101469-29-8]. (*Malonic dihydrazide*)*zinc nitrate*
Cryst. + $2H_2O$.

Bis-sulfate: [58551-17-0].
Cryst. + $2H_2O$ (H_2O). Struct. consists of discrete dinuclear cations, $SO_4^{2\ominus}$, and uncoord. H_2O: strong H-bonds.

[62747-23-3, 69878-60-0]

Shvelashvili, A.E. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1976, **21**, 159 (*cryst struct, sulfate*)
Machkhoshvili, R.I. *et al, Koord. Khim.*, 1977, **3**, 332 (*synth, ir, thermal dec*)
Shvelashvili, A.E. *et al, Soobshch. Akad. Nauk. Gruz. SSR*, 1985, **119**, 529 (*synth, ir, nitrate*)

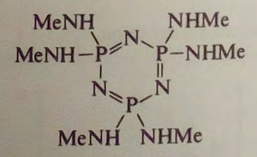
IC-005527

$C_6H_{24}N_9P_3$

2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexakis(methylamino)-1,3,5,2,4,6-triazatriphosphorine, 9CI

2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexakis(methylamino) cyclotriphosphazene. 2,2,4,4,6,6-Hexakis(methylamino)-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2,4,4,6,6-Hexakis(methylamino)-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine

[1635-63-8]



M 315.2

Cryst. ($CHCl_3$/pet. ether). Mp 258-259°.

Ray, S.K. *et al, J. Chem. Soc.*, 1961, 872 (*synth*)
Allcock, H.R. *et al, Inorg. Chem.*, 1977, **16**, 3362 (*props*)
Allcock, H.R. *et al, J. Am. Chem. Soc.*, 1981, **103**, 2250.
Allcock, H.R. *et al, J. Org. Chem.*, 1981, **46**, 13 (*P-31 nmr*)
Allcock, H.R. *et al, Inorg. Chem.*, 1982, **21**, 515 (*P-31 nmr, props*)

IC-005528

$C_6H_{24}N_{12}NiS_6^{2\oplus}$

Hexakis(thiourea)nickel(*II*)(2+), 8CI

[32594-32-4]

$[Ni[S{=}C(NH_2)_2]_6]^{2\oplus}$

M 515.4 (ion)
Ligand binds through S only. Paramagnetic.

Dibromide: [14976-06-8].
$C_6H_{24}Br_2N_{12}NiS_6$ M 675.2
Green cryst. Sol. EtOH, Me_2CO.

Diperchlorate: [15292-38-3].
$C_6H_{24}Cl_2N_{12}NiO_8S_6$ M 714.3
Green solid. Sol. MeOH, Me_2CO.

Dinitrate: [15006-81-2].
$C_6H_{24}N_{14}NiO_6S_6$ M 639.4
Yellow-green cryst. Sol. Me_2CO.

Cotton, F.A. *et al, Inorg. Chem.*, 1964, **3**, 17 (*synth, ir, uv, elec cond, magnetism*)
Flint, C.D. *et al, J. Chem. Soc. A*, 1966, 744 (*synth, ir*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1967, 884 (*ir*)
Weininger, M.S. *et al, Inorg. Chem.*, 1969, **8**, 424 (*cryst struct*)
Eaton, D.R. *et al, Can. J. Chem.*, 1975, **53**, 633 (*pmr*)
Srinivasan, V. *et al, Inorg. Chim. Acta*, 1977, **25**, L85 (*pe*)

IC-005529

$C_6H_{24}N_{12}O_6Ti^{3\oplus}$

Hexakis(urea-*O*)titanium(3+), 11CI

Hexaureatitanium(III)(*3+*)

[45284-50-2]

$[Ti[O{=}C(NH_2)_2]_6]^{3\oplus}$

M 408.2 (ion)

Trigonally distorted octahedron. Synth. by adding $TiCl_3$ to an aq. soln. of urea followed by K salt of the anion or from $TiCl_3$ and urea in EtOH. Paramagnetic.

Trichloride: [22869-81-4].
$C_6H_{24}Cl_3N_{12}O_6Ti$ M 514.5

Triiodide: [15002-29-6].
$C_6H_{24}I_3N_{12}O_6Ti$ M 788.9
Deep blue solid (EtOH). μ_{eff} = 1.63μ_B (300K), 1.50 μ_B (77K).

Triperchlorate: [15189-70-5].
$C_6H_{24}Cl_3N_{12}O_{18}Ti$ M 706.5
Deep blue solid (EtOH).

Machin, D.J. *et al, J. Chem. Soc. A*, 1968, 195 (*synth, magnetism*)
Davis, P.H. *et al, Inorg. Chem.*, 1970, **9**, 1111 (*cryst struct*)
Figgis, B.N. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 187 (*cryst struct, magnetism*)
Figgis, B.N. *et al, Aust. J. Chem.*, 1972, **25**, 2233 (*cryst struct, magnetism*)
Geio-Blazekova, M., *Z. Anorg. Allg. Chem.*, 1973, **402**, 1 (*synth, magnetism, uv-vis, chloride*)
Pickering, M., *J. Chem. Educ.*, 1985, **62**, 442 (*synth*)

IC-005530

$C_6H_{24}N_{12}O_6V^{3\oplus}$

Hexakis(urea-*O*)vanadium(*III*)(3+), 11CI

[22624-26-6]

$V[O{=}C(NH_2)_2]_6^{3\oplus}$ (O_h)

M 411.2 (ion)

Tribromide: [19319-49-4]. *Vanadium*(III) *bromide hexaurea*
Synth. by electrolytic reduction of a soln. of V_2O_5 in HBr then addition of urea. Green cryst. + $3H_2O$, readily dehydrates at r.t. to pale green solid. Paramagnetic; μ_{eff} = 2.75 μ_B (300K), 2.68 μ_B (78K).

Triiodide: [38581-19-0]. *Vanadium*(III) *iodide hexaurea*
Synth. by electrolytic reduction of $VO(SO_4)$ then addition of urea and KI. Green cryst. Paramagnetic; μ_{eff} = 2.83μ_B (300K), 2.32μ_B (4.2K).

Triperchlorate: [18581-56-1]. *Vanadium*(III) *perchlorate hexaurea*
Synth. as for the iodide. Green solid. Paramagnetic; μ_{eff} = 2.71μ_B (300K), 2.67μ_B (86K).
▷ Potentially explosive.

Carlin, R.L. *et al, J. Chem. Phys.*, 1967, **47**, 4901 (*synth, magnetism, bromide*)
Figgis, B.N. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2182 (*synth, magnetism, iodide*)
Baker, J. *et al, Aust. J. Chem.*, 1980, **33**, 2377 (*magnetism, perchlorate*)

IC-005531

$C_6H_{24}N_{12}O_6Zn^{2\oplus}$

Hexakis(urea-*O*)zinc(2+)

Hexaureazinc(2+)

$[Zn[O{=}C(NH_2)_2]_6]^{2\oplus}$

M 425.7 (ion)

Distorted octahedral Zn.

Bis-tetrafluoroborate: [50937-46-7].
Cryst. Mp 190°, Mp 138° dec.

Diperchlorate: [59272-46-7].
Colourless prisms. Mp 142°.
▷ Potentially explosive.

Dinitrate: [38625-10-4].
Cryst. Extensively H-bonded in solid state.

Sulfate: [15025-10-2].
$C_6H_{24}N_{12}O_{10}SZn$ M 521.7
Cryst. Forms a monohydrate. H-bonds between H_2O and urea and between H_2O and $SO_4^{2\ominus}$ in solid.

[106207-99-2]

Diushenalieva, N. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1961, **6**, 980 (*synth*)
Van de Giesen, W. *et al, Cryst. Struct. Commun.*, 1972, **1**, 257 (*cryst struct, nitrate*)
de Bolster, M.W.G. *et al, Inorg. Chim. Acta*, 1973, **7**, 439 (*synth, tetrafluoroborate*)
Molchanov, Ya.Ya. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1976, **21**, 476; 1977, **22**, 1760, 3230 (*synth, ir, perchlorate*)
Zhou, Z. *et al, Huaxue Xuebao*, 1986, **44**, 1045; *CA*, **106**, 41886 (*cryst struct, sulfate*)

IC-005532

$C_6H_{24}N_{12}OsS_6^{2\oplus}$

Hexakis(thiourea)osmium(*II*)(2+)

$[Os[S{=}C(NH_2)_2]_6]^{2\oplus}$

M 646.9 (ion)

Intermediate in reaction between OsO_4 and thiourea.

Sulfate: Synth. from $[OsO_2(NH_2CSNH_2)_4]^{2\oplus}$ in $SO_4^{2\ominus}$ soln. Yellow-brown solid. Dec. in H_2O or dil. acid to give $Os(OH)_4$.

Sauerbrunn, R.D. *et al, J. Am. Chem. Soc.*, 1953, **75**, 3554 (*synth*)

IC-005533

$C_6H_{24}N_{12}OsS_6^{3\oplus}$

Hexakis(thiourea)osmium(*III*)(3+)

[12300-37-7]

$[Os[S{=}C(NH_2)_2]_6]^{3\oplus}$

M 646.9 (ion)

Has only been observed as an ion in soln. Obt. by reaction of thiourea with OsO_4 in acidic medium.

Sauerbrunn, R.D. *et al, J. Am. Chem. Soc.*, 1953, **75**, 3554 (*synth*)

IC-005534

$C_6H_{24}N_{12}PbS_6^{2\oplus}$

Hexakis(thiourea)lead(*II*)(2+)

[45283-97-4]

$[Pb[S{=}C(NH_2)_2]_6]^{2\oplus}$

M 663.9 (ion)

Dinitrate: [13985-93-8].
Synth. from $Pb(NO_3)_2$ + thiourea. Cryst.
Diperchlorate: [17500-46-8].
Synth. from $Pb(ClO_4)_2$ + thiourea. Yellow needles (tetragonal) or white needles (triclinic). Sol. H_2O.

Rosenheim, A. *et al*, *Z. Anorg. Allg. Chem.*, 1906, **49**, 13 (*synth, nitrate*)
Mahr, C. *et al*, *Justus Liebigs Ann. Chem.*, 1939, **542**, 44 (*synth, perchlorate*)
Boeyens, J.C.A. *et al*, *Nature (London)*, 1966, **211**, 588 (*cryst struct*)
Boeyens, J.C.A. *et al*, *Inorg. Chem.*, 1967, **6**, 1408 (*cryst struct*)
Gosavi, R.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1937 (*ir*)
Goldberg, I. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 400 (*cryst struct, perchlorate*)

$C_6H_{24}N_{12}RuS_6^{3\oplus}$ IC-005535

Hexakis(thiourea-*S*)ruthenium(*III*)(3+), 9CI

[45284-04-6]

$$Ru[S{=}C(NH_2)_2]_6^{3\oplus}(O_h)$$

M 557.8 (ion)
Tetraiodomercuriate(II)(*2:3*):
$C_{12}H_{48}Hg_3I_{12}N_{24}Ru_2S_{12}$ M 3240.2
Green-black solid. μ_{eff} = 2.0μ_B; Ir $\nu_{C=S}$ 685 cm^{-1}.

Youmans, H.L., *Inorg. Chem.*, 1970, **9**, 669 (*synth, ir, magnetism*)

$C_6H_{24}N_{12}S_6Tc^{3\oplus}$ IC-005536

Hexakis(thiourea-*S*)technetium(*III*)(3+), 11CI

[91042-52-3]

$$[Tc[S{=}C(NH_2)_2]_6]^{3\oplus}$$

M 555.6 (ion)
Octahedral. Synth. from $TcO_4^{\ominus}$ + thiourea in ethanolic HCl. Valuable synthetic intermediate.
Trichloride: [91467-29-7]. *Technetium*(III) *chloride hexakis-thiourea*
$C_6H_{24}Cl_3N_{12}S_6Tc$ M 661.9
Deep red solid + $4H_2O$ (aq. HCl/thiourea). Sol. MeOH; spar. sol. EtOH. Mp 174° dec. Dec. in H_2O.
Tris-tetrafluoroborate: [91467-31-1].
Orange-red solid. Sol. MeOH, EtOH, Me_2CO, MeCN. Mp 178-180° dec.

Abrams, M.J., *J. Labelled Compd. Radiopharm.*, 1982, **14**, 1596 (*synth*)
Abrams, M.J. *et al*, *Inorg. Chem.*, 1984, **23**, 3284 (*synth, cryst struct, ir, uv, props, magnetism*)
Münze, R. *et al*, *J. Radioanal. Nucl. Chem.*, 1984, **86**, 79 (*uv, electrophoresis*)
Spies, H. *et al*, *Inorg. Chim. Acta*, 1985, **109**, L3 (*use*)
Bandoli, G. *et al*, *Inorg. Chim. Acta*, 1987, **132**, 177 (*use*)
Hashimoto, M. *et al*, *J. Radioanal. Nucl. Chem.*, 1991, **153**, 283 (*use, kinetics*)

$C_6H_{24}NiO_6^{2\oplus}$ IC-005537

Hexakis(methanol)nickel(*II*)(2+)

$$[Ni(MeOH)_6]^{2\oplus}(O_h)$$

M 250.9 (ion)
Starting material for synth. of Ni complexes.
Diperchlorate: [14100-07-3]. *Nickel*(II) *perchlorate hexakis-methanol*
$C_6H_{24}Cl_2NiO_{14}$ M 449.8
Yellow green hygroscopic powder. Mp 146°.
▷ Potentially explosive.
Bis-tetrafluoroborate: [36051-19-1]. *Nickel*(II) *tetrafluoroborate hexakis-methanol*
$C_6H_{24}B_2F_8NiO_6$ M 424.5
Hygroscopic light green solid. Mp 157°.
Dinitrate: [36051-25-9]. *Nickel*(II) *nitrate hexakis-methanol*
$C_6H_{24}N_2NiO_{12}$ M 374.9
Light green solid. Mp 63°.

Luz, Z. *et al*, *J. Chem. Phys.*, 1964, **40**, 1066 (*uv-vis*)
Imhof, V. *et al*, *Inorg. Chem.*, 1965, **4**, 427 (*synth, uv-vis, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 57, 1968, **C1**, 486 (*rev*)
Van Ingen Schenau, A.D. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1972, **91**, 88 (*synth, uv-vis, ir*)

$C_6H_{24}O_6V^{2\oplus}$ IC-005538

Hexakis(methanol)vanadium(*II*)(2+), 11CI

$$[V(OHMe)_6]^{2\oplus}(O_h)$$

M 243.1 (ion)
Octahedral ethanol analogue known. Bis- and tetrakis(methanol) adducts can also be obt.
Dichloride: [96328-54-0]. *Vanadium*(II) *chloride hexakis(methanol)*
$C_6H_{24}Cl_2O_6V$ M 314.0
Synth. from $[V_2(THF)_6Cl_3]^{\oplus}$ and MeOH. Purple-blue cryst.
Dibromide: [21655-23-2]. *Vanadium*(II) *bromide hexakis(methanol)*
$C_6H_{24}Br_2O_6V$ M 403.0
Synth. by electrolytic reduction of VBr_3 in MeOH/HBr. Purple solid. Paramagnetic; μ_{eff} = 3.97μ_B (92K); 3.98μ_B (298K).

Seifert, H.J. *et al*, *Z. Anorg. Allg. Chem.*, 1968, **360**, 50 (*synth, uv-vis, magnetism, bromide*)
Cotton, F.A. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 3850 (*synth, cryst struct, uv-vis, chloride*)

$C_6H_{24}O_6Zn^{2\oplus}$ IC-005539

Hexakis(methanol-*O*)zinc(2+)

$$[Zn(MeOH)_6]^{2\oplus}$$

M 257.6 (ion)
Octahedral cation. Salts synth. from $[Zn(OH_2)_6]X_2$ and $(MeO)_3CH$.
Bis-tetrafluoroborate: [36051-20-4].
White cryst. Insol. Et_2O, pentane, C_6H_6. Mp 114°.
Dinitrate: [36051-26-0].
White cryst. Mp ~35°.
Diperchlorate: [36158-49-3].
White cryst. Mp 115°.
▷ Potentially explosive.

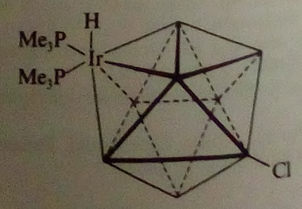
van Ingen Schenau, A.D. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1972, **91**, 88 (*synth, ir*)

$C_6H_{26}B_8ClIrP_2$ IC-005540

[(3,4,5,6,7,8-η)-1-Chloro-2,3,4,5,7,8-heptahydrooctaborato(4−)]hydrobis(trimethylphosphine) iridium, 11CI

1,1,1-Bis(trimethylphosphine)hydrido-8-chloro-1-iridanonaborane(*8*)

[82447-28-7]



M 474.3
iso-closo-. Air-stable poppy-red solid (by tlc).

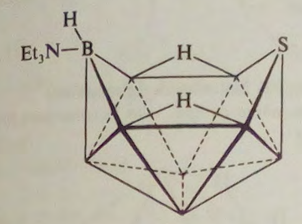
Bould, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 346 (*cryst struct, synth, pmr*)
Baker, R.T. *et al*, *Inorg. Chem.*, 1986, **25**, 109 (*rev*)

$C_6H_{26}B_9NS$ IC-005541

9-Triethylamine-6-thiadecaborane(11)

Thiadecaborane(11) compd. with triethylamine (1:1), 8CI. 6-Thiadecaborane(11) compd. with diethylethanamine (1:1), 10CI

[12551-35-8]



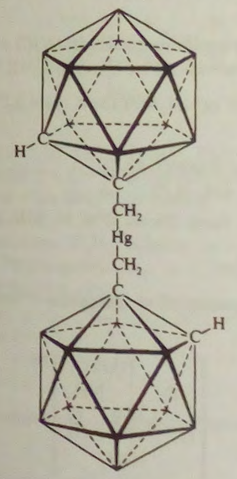
M 241.6
arachno-. Pale yellow cryst. (C_6H_6). Sol. MeCN. Mp 111-113°. Subl. *in vacuo*.

Hertler, W.R. *et al*, *Inorg. Chem.*, 1967, **6**, 1696 (*synth, uv, ir, pmr, B-11 nmr*)
Hilty, T.K. *et al*, *Inorg. Chem.*, 1979, **18**, 1106 (*cryst struct*)

$C_6H_{26}B_{20}Hg$ IC-005542

Bis(1,2-dicarbadodecaboran(12)-1-ylmethyl)mercury, 8CI

Bis(o-carboranylmethyl)mercury. Bis(barenylmethyl)mercury



M 515.0
Cryst. (C_6H_6/hexane). Mp 280-282° dec.

Zakharkin, L.I. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 664 (*synth*)

$C_6H_{26}B_{20}Hg$ IC-005543

Bis(2-methyl-1,2-dicarbadodecaboran(12)-1-yl)mercury, 10CI, 8CI

Bis(methyl-o-carboranyl)mercury. Bis(methylbarenyl) mercury

[23940-18-3]

As Bis(1,2-dicarbadodecaboran(12)-1-yl)mercury, IC-004476 with

R = CH_3

M 515.0
Cryst. (cyclohexane). Mp 255-256°.
Bipy complex: [18116-69-3].
$C_{16}H_{34}B_{20}HgN_2$ M 671.2
Cryst. Mp 252-254°.

Zakharkin, L.I. *et al*, *J. Organomet. Chem.*, 1965, **4**, 211 (*synth*)
Bregadze, V.I. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1967, **177**, 1021 (*deriv*)
Berberova, N.T. *et al*, *Zh. Obshch. Khim.*, 1977, **47**, 726 (*electrochem*)
Zakharkin, L.I. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1984, **33**, 1087 (*synth*)

$C_6H_{26}B_{20}Hg$ IC-005544

Bis(7-methyl-1,7-dicarbadodecaboran(12)-1-yl)mercury, 8CI

*Bis(methyl-*m*-carboranyl)mercury. Bis(methylneobarenyl) mercury*

[12106-95-5]

As Bis(1,7-dicarbadodecaboran(12)-1-yl)mercury, IC-004478 with

R = CH_3

M 515.0
Cryst. (hexane). Mp 185-186°, Mp 191-192°.

Zakharkin, L.I. *et al*, *J. Organomet. Chem.*, 1967, **7**, 385 (*synth*)
Stanko, V.I. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1968, 414 (*electrochem*)

$C_6H_{26}CrN_6O_2^{3\oplus}$ IC-005545

Tetraamminebis(*N*,*N*-dimethylformamide-*O*) chromium(*III*)(3+), 10CI

$$[Cr(O{=}CHNMe_2)_2(NH_3)_4]^{3\oplus}$$

M 266.3 (ion)
Octahedral cation. Many related solvo complexes, also of DMSO, used in further syntheses.

cis-form

Triperchlorate: [78549-83-4].
Synth. from *cis*-$[Cr(OH_2)_2(NH_3)_4](ClO_4)_3$ in DMF. Cryst. (aq. $NaClO_4$).

trans-form

Triperchlorate: [72382-33-3].
Synth. from *trans*-$[Cr(OH_2)_2(NH_3)_4](ClO_4)_3$ in DMF. Purple cryst. (aq. $HClO_4$).

Jackson, W.G. *et al*, *Inorg. Chim. Acta*, 1977, **22**, 111 (*synth*)
Casabó, J. *et al*, *Inorg. Chim. Acta*, 1979, **36**, 183 (*synth, uv, solvol*)
Riccieri, P. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 739 (*synth, uv, ir*)

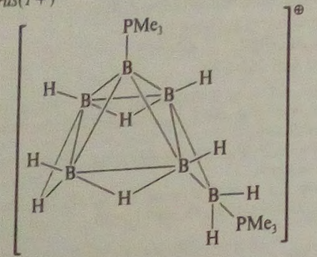
IC-005546

$C_6H_{27}B_6P_2^{\oplus}$

Bis(trimethylphosphine)nonahydrohexaboron(1+)

3,6-Bis(trimethylphosphine)hexaborane(10) (1+).

Trimethyl[nonahydro(trimethylphosphine)hexaborato(1−)]phosphorus(1+)



M 226.0 (ion)

arachno-basal bridged square pyramid; one of alternative 'arachno' structures for B_6 clusters.

Tetrafluoroborate: [110795-78-3].
Colourless cryst. (CH_2Cl_2); stable at −80°, dec. slowly at 0°. Sol. CH_2Cl_2.

[110795-79-4]

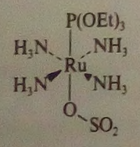
Kameda, M. *et al, Inorg. Chem.*, 1987, **26**, 3968 (*synth, pmr, B-11 nmr, P-31 nmr*)

IC-005547

$C_6H_{27}N_4O_6PRuS$

Tetraammine[sulfito(2−)-*O*](triethyl phosphite-*P*)ruthenium(*II*)

[64939-22-6]



M 415.4

trans-Octahedral. Prepd. by treating Tetraammineaqua(triethyl phosphite-*P*)ruthenium(*II*)(2+), IC-005552 with sulfite. Only obsd. in soln. Sol. H_2O.

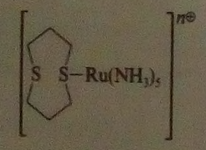
Franco, D.W. *et al, Inorg. Chem.*, 1978, **17**, 571 (*synth, uv*)

IC-005548

$C_6H_{27}N_5RuS_2^{2\oplus}$

Pentaammine(1,5-dithiocane-S^1)ruthenium(*II*)(2+), 10CI

[66100-87-6]



n = 2

M 334.5 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with a excess of 1,5-dithiocane. Sol. H_2O, Me_2CO.

Bis-hexafluorophosphate: Yellow solid.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electrochem*)

IC-005549

$C_6H_{27}N_5RuS_2^{3\oplus}$

Pentaammine(1,5-dithiocane-S^1)ruthenium(*III*)(3+), 10CI

[66100-86-5]

As Pentaammine(1,5-dithiocane-S^1)ruthenium(*II*)(2+), IC-005548 with

n = 3

M 334.5 (ion)

Prepd. by oxidation of the Ru(*II*) analogue with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al, J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electrochem*)

IC-005550

$C_6H_{28}B_6P_2$

Hexaborane(10) bis(trimethylphosphine)

Trimethylphosphine compd. with hexaborane(10) (2:1)

[57034-29-4]

M 227.1

Stable *hypho*-cage structure. Monoclinic cryst. Sol. CH_2Cl_2, THF. Mp 125° dec.

Mangion, M. *et al, J. Am. Chem. Soc.*, 1976, **98**, 449 (*synth, cryst struct, nmr*)

IC-005551

$C_6H_{29}CoN_7O^{3\oplus}$

Pentakis(methylamine)ureacobalt(*III*)(3+)

Pentakis(methanamine)(urea-O)cobalt(III)(3+), 11CI

$[Co(NH_2Me)_5O{=}C(NH_2)_2]^{3\oplus}$

M 274.2 (ion)

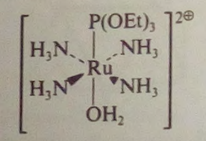
Dithionate (2:3): [100681-43-4].
Purple solid. Sol. H_2O.

Curtis, N.J. *et al, Inorg. Chem.*, 1986, **25**, 1033 (*synth, uv, kinetics*)

IC-005552

$C_6H_{29}N_4O_4PRu^{2\oplus}$

Tetraammineaqua(triethyl phosphite-*P*)ruthenium(*II*)(2+)



M 353.3 (ion)

trans-Octahedral isomer only. Sol. H_2O.

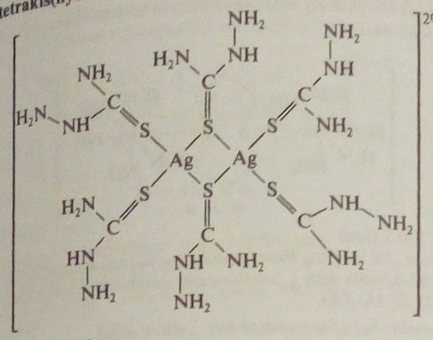
Bis-trifluoromethylsulfonate: [64939-04-4].
Prepd. by treating Tetraamminebis(triethyl phosphite-*P*)ruthenium(*II*)(2+), IC-008343 with aq. F_3CSO_3H at r.t.

Franco, D.W. *et al, Inorg. Chem.*, 1978, **17**, 571 (*synth, uv*)

IC-005553

$C_6H_{30}Ag_2N_{18}S_6^{2\oplus}$

Bis[μ-(hydrazinecarbothioamide-*S:S*)]tetrakis(hydrazinecarbothioamide-*S*)disilver(2+), 12CI



M 762.5 (ion)

Dichloride: [108089-43-6].
Cryst.

Nardelli, M. *et al, Ric. Sci.*, 1965, **35**, 480 (*synth*)
Bonamartini, A.C. *et al, Acta Crystallogr., Sect. C*, 1987, **43**, 407 (*struct*)

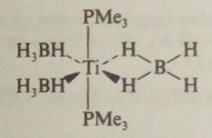
IC-005554

$C_6H_{30}B_3P_2Ti$

Tris(tetrahydroborato)bis(trimethylphosphine)titanium(*III*)

Bis[tetrahydroborato(1−)-H][tetrahydroborato(1−)-H,H']bis(trimethylphosphine)titanium, 11CI

[106245-63-0]



M 244.5

Prepd. by reaction of $TiCl_4$, $LiBH_4$, PMe_3 in Et_2O. Possible model for C—H bond activation in CH_4 (isoelectronic with $BH_4^{\ominus}$) at metals. V. air-sensitive blue cryst. (pentane at −20°); stable under argon for several days. Sol. pentane, C_6H_6, toluene. Ir ν_{BH4} 2532, 2401, 2358 cm^{-1}. Paramagnetic, μ_{eff} = 1.7μ_B; dec. at 104°. Relat. compds. also obt.

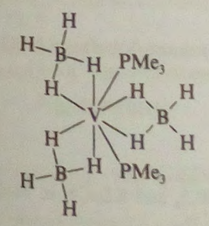
Jensen, J.A. *et al, J. Am. Chem. Soc.*, 1988, **110**, 4977 (*synth, ir, pmr, esr, cryst struct*)

IC-005555

$C_6H_{30}B_3P_2V$

Tris[tetrahydroborato(1−)-*H,H'*]bis(trimethylphosphine)vanadium

[114692-85-2]



M 247.6

Has nearly ideal D_{3h} geometry expected for non-degenerate d^2 sp. Paramagnetic, bright-green cryst. (pentane). Sol. C_6H_6, pentane, Et_2O. Mp 94° dec. Ir *v* 2431s, 2385s, 2227s, 2218w, 2087s, 1951w cm^{-1}. μ_{eff} = 2.5μ_B.

Jensen, J.A. *et al, J. Am. Chem. Soc.*, 1988, **110**, 4450 (*synth, cryst struct, ir, pmr, magnetism*)
Jensen, J.A. *et al, Inorg. Chem.*, 1989, **28**, 2114 (*synth, ir, pmr, esr, magnetism, cryst struct*)

IC-005556

$C_6H_{30}CrN_6^{3\oplus}$

Hexakis(methylamine)chromium(*III*)

Hexakis(methanamine)chromium(3+), 10CI

[33914-82-8]

$[Cr(NH_2Me)_6]^{3\oplus}$

M 238.3 (ion)

Octahedral geometry about Cr. Acidopentamine cations, e.g. Chloropentakis(methylamine)chromium(*III*)(2+), IC-004812 are formed in inorg. acids.

Tribromide: [61475-80-7].
Yellow.

Trinitrate: [19223-31-5].
Yellow.

Triperchlorate: [61475-81-8].
Yellow.

Parris, M. *et al, Inorg. Nucl. Chem. Lett.*, 1967, **3**, 337 (*synth*)
Garner, C.S. *et al, Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Kuhn, K. *et al, J. Phys. Chem.*, 1981, **85**, 665.
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 787 (*rev*)

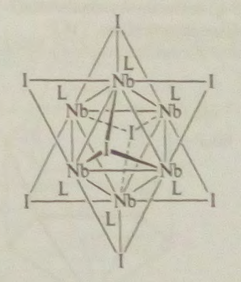
IC-005557

$C_6H_{30}I_8N_6Nb_6$

Octa-μ_3-iodohexakis(methylamine)hexaniobium

Octa-μ_3-iodo-hexakis[(methylamine)niobium]. Octa-μ_3-iodohexakis(methanamine)hexaniobium, 11CI. Hexaniobium octaiodide hexakis(methylamine)

[93683-43-3]



L = NH_2Me

M 1759.0

Synth. from Nb_6I_{11} and $MeNH_2$ in EtOH. The formal oxidation state of Nb in this compd. is unusually low. Dark red air-sensitive solid.

▷ A second, amorphous, product is formed in this synth. which is pyrophoric when dry.

Stollmaier, F. *et al, Inorg. Chem.*, 1985, **24**, 168 (*synth, cryst struct*)

IC-005558

$C_6H_{30}MnN_6^{2\oplus}$

Hexakis(methylamine)manganese(*II*)(2+)

Hexakis(methanamine)manganese(2+), 11CI

$[Mn(NMeH_2)_6]^{2\oplus}$

M 241.2 (ion)

Complexes $[Mn(MeNH_2)_6]X_2$ are formed by passing $MeNH_2$ over anhydrous MnX_2 salts or $MeNH_2$ into aq. $MnSO_4$ buffered with $(NH_4)_2SO_4$.

Dichloride: [85295-03-0]. *Manganese*(II) *chloride hexakis-methylamine*
$C_6H_{30}Cl_2MnN_6$ M 312.1
Synth. from $MnCl_2$ and $MeNH_2$.

Chromate(2−): [15693-84-2].
Synth. by shaking $MnCrO_4$ and $MeNH_2$ in a 1:6 ratio in EtOH for 3 d. $\mu_{eff} = 5.89\mu_B$.

Narain, G. *et al*, *J. Indian Chem. Soc.*, 1966, **43**, 694 (*synth, ir, magnetism*)
Skukla, P., *J. Prakt. Chem.*, 1968, **38**, 253 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 21 (*rev, bibl*)

$C_6H_{30}N_6Ru^{2\oplus}$ IC-005559

Hexakis(methylamine)ruthenium(*II*)(2+)
Hexakis(methanamine)ruthenium(2+), *9CI*
[45047-33-4]

$[Ru(NH_2Me)_6]^{2\oplus}$

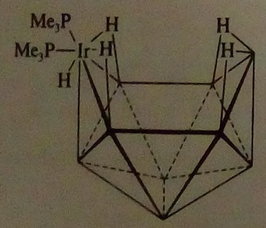
M 287.4 (ion)
Prepd. by reducing $RuCl_3.xH_2O$ with Zn/Hg in the presence of $MeNH_2$.

Dibromide:
$C_6H_{30}Br_2N_6Ru$ M 447.2
Yellow salt.
Diiodide: Yellow salt.
Bis-tetrafluoroborate: Yellow salt.

McWhinnie, W.R. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 461 (*synth, ir, uv*)
Miller, J.D. *et al*, *Inorg. Chim. Acta*, 1975, **12**, 267 (*synth, catalysis*)

$C_6H_{32}B_9IrP_2$ IC-005560

Hydro[(4,8,9-η)-tridecahydrononaborato(2−)-H^8,H^9] bis(trimethylphosphine)iridium, 11CI
6,6,6-(Hydrido)bis(trimethylphosphine)-6-iridadecaborane(*13*)
[82090-18-4]

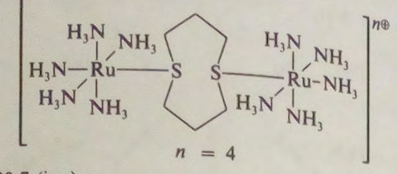


M 455.7
nido-. Air-stable yellow cryst. (by tlc. CH_2Cl_2/ pet. ether 1:1). V. sol. CH_2Cl_2, $CHCl_3$.

Boocock, S.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 713 (*synth, deriv, struct, B-11 nmr, pmr, P-31 nmr*)
Bould, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 1903 (*synth*)

$C_6H_{42}N_{10}Ru_2S_2^{4\oplus}$ IC-005561

Decaammine[μ-(1,5-dithiocane-S^1:S^5)]diruthenium(*II*) (4+), 10CI
μ-(1,5-Dithiocane)-bis[pentammineruthenium(II)]
[66083-94-1]



n = 4

M 520.7 (ion)
Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with 1,5-dithiocane stoichiometrically. Sol. H_2O, Me_2CO.

Tetrakis-hexafluorophosphate: Yellow solid.

Stein, C.A. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electrochem*)

$C_6H_{42}N_{10}Ru_2S_2^{5\oplus}$ IC-005562

Decaammine[μ-(1,5-dithiocane-S^1:S^5)]diruthenium(*II,III*) (5+), 10CI
μ-(1,5-Dithiocane)-bis[pentaammineruthenium(II,III)]
[66402-84-4]

As Decaammine[μ-(1,5-dithiocane-S^1:S^5)]diruthenium(*II*) (4+), IC-005561 with

n = 5

M 520.7 (ion)
Prepd. by oxidizing Decaammine[μ-(1,5-dithiocane-S^1:S^5)] diruthenium(*II*)(4+), IC-005561 with Ce(*IV*). Not isol. Sol. H_2O, Me_2CO.

Stein, C.A. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 1635 (*synth, uv, electrochem*)

$C_6HfN_6O_6^{2\ominus}$ IC-005563

Hexakis(cyanato-*N*)hafnate(*IV*)(2−), 9CI
Hexaisocyanatohafnate(IV)(2−)

$[Hf(NCO)_6]^{2\ominus}$

M 430.5 (ion)
Octahedral. The *N*-bonding of the isocyanate has been deduced from vibrational spectra.

Bis-Et_4N salt: [40418-96-0].
Synth. from $HfCl_4$ and $[Et_4N]NCO$ in MeCN followed by freshly prepd. AgNCO. White hygroscopic solid. Sol. MeCN.

Peterson, E.J. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 241 (*synth, ir, raman*)

$C_6HfN_6Se_6^{2\ominus}$ IC-005564

Hexakis(selenocyanato-*N*)hafnate(*IV*)(2−), 9CI
Hexaisoselenocyanatohafnate(IV)(2−)

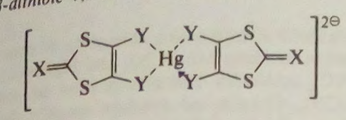
$[Hf(NCSe)_6]^{2\ominus}$

M 808.3 (ion)
Di-K salt: [34445-22-2].
Synth. from $HfCl_4$ and KSeCN in MeCN. Tan-coloured solid. Sol. MeCN.

Galliart, A. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 3568 (*synth, ir, uv-vis*)

$C_6HgO_2S_8^{2\ominus}$ IC-005565

Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-S^4,S^5] mercurate(2−), 12CI
Bis(4,5-dimercapto-1,3-dithiole-2-onato)mercurate(2−). *Bis(2-oxo-1,3-dithiole-4,5-dithiolato)mercurate*(2−)



X = O, Y = S

M 561.1 (ion)
Bis-tetrabutylammonium salt: [119797-54-5].
Red cryst. Dec. at 98-102°.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **567**, 131 (*synth, ir, cmr*)

$C_6HgS_6Se_4^{2\ominus}$ IC-005566

Bis[4,5-diselenyl-1,3-dithiole-2-thionato(2−)-*Se*,*Se'*] mercurate(2−), 12CI
Bis(2-thio-1,3-dithiole-4,5-diselenolato)mercurate(2−)

As Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-S^4,S^5] mercurate(2−), 12CI, IC-005565 with

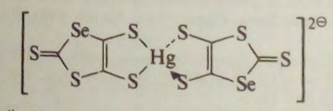
X = S, Y = Se

M 780.8 (ion)
Bis-tetrabutylammonium salt: [120752-56-9].
Red cryst. Sol. $CHCl_3$, DMSO. Mp 137-138° dec.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1989, **577**, 206 (*synth, ir, uv-vis, cmr*)
Olk, B. *et al*, *Z. Chem.*, 1989, **29**, 64 (*Se-77 nmr*)

$C_6HgS_8Se_2^{2\ominus}$ IC-005567

Bis(1,3-thiaselenole-2-thione-4,5-dithiolato) mercurate(2−)
Bis[4,5-dimercapto-1,3-thiaselenole-2-thionato(2−)-S^4,S^5] *mercurate*(2−)



M 687.1 (ion)
Bis-tetrabutylammonium salt: [130726-31-7].
Dark violet cryst. (MeOH). Sol. $CHCl_3$. Dec. at 150-153°.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1990, **581**, 59 (*synth, ir, cmr, uv*)

$C_6HgS_{10}^{2\ominus}$ IC-005568

Bis[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-S^4,S^5] mercurate(2−), 11CI

As Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-S^4,S^5] mercurate(2−), 12CI, IC-005565 with

X = Y = S

M 593.3 (ion)
Bis-tetrabutylammonium salt: Red cryst. (EtOH). Mp 146.5-154° dec.
1,1'-Dimethyl-4,4'-bipyridinium(2+) *salt:* [107769-60-8].
Brown-violet needles. Mp 205°.
[85920-62-3]

Wawzonek, S. *et al*, *J. Electrochem. Soc.*, 1983, **130**, 803 (*synth, ir, pmr, cmr, ms*)
Lahner, S. *et al*, *Chem. Ber.*, 1987, **120**, 1011 (*synth, uv-vis*)
Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **567**, 131 (*synth, cmr, ir*)

$C_6Ho_2O_{12}$ IC-005569

Holmium(*III*) oxalate
Tris(oxalato)diholmium. Tris(ethanedioato)diholmium
[3269-15-6]

$Ho_2(C_2O_4)_3$

M 593.9
Decahydrate: [28965-57-3].
$C_6H_{20}Ho_2O_{22}$ M 774.0
Yellow solid. Several other hydrates also reported.
[13266-79-0, 35139-25-4, 35139-27-6, 58176-70-8]

Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth, tga*)
Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Hansson, E., *Acta Chem. Scand.*, 1973, **27**, 823 (*struct*)
Sharov, V.A. *et al*, *Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Jeyaraj, G.L. *et al*, *Thermochim. Acta*, 1983, **71**, 345 (*tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6I_4O_6Os_2$ IC-005570

Hexacarbonyldi-μ-iododiiododiosmium
Hexacarbonyltetraiododiosmium
[17632-08-5]

As Di-μ-bromodibromohexacarbonyldiosmium, IC-004864 with

X = I

M 1056.0
Synth. by exchange between chloro-derivative and LiI in Me_2CO. Yellow cryst. (C_6H_6).

Hales, L.A.W. *et al*, *J. Chem. Soc. A*, 1967, 1932 (*synth, uv*)
Psaro, R. *et al*, *J. Organomet. Chem.*, 1981, **213**, 215 (*synth, ir*)

$C_6InN_6S_6^{3\ominus}$ IC-005571

Hexakis(thiocyanato-*N*)indate(3−)
Hexa(isothiocyanato)indate(III)(3−)

$[In(NCS)_6]^{3\ominus}$ (O_h)

M 463.3 (ion)
Tris-Me_4N salt: [23759-19-5].
Synth. from $InCl_3$, KSCN and $[Me_4N]SCN$ in EtOH. White cryst. Spar. sol. EtOH.
Tris-Ph_4As salt: [60385-97-9].
Obt. by recrystallisation of $[Ph_4As]In(NCS)_5$ from Me_2CO. Colourless cryst. (Me_2CO).

Schmidtke, H. *et al*, *Z. Naturforsch., A*, 1969, **24**, 126 (*synth, uv-vis*)
Habeeb, J.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 96 (*synth*)
Einstein, F.W.B. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 2234 (*cryst struct*)
Mal'tseva, V.S., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 1720 (*ir*)

IC-005572

$C_6InO_{12}^{3\ominus}$

Tris(oxalato)indate(3−)

Tris[ethanedioato(2−)-O,O']indate(3−), 9CI

[60308-06-7]

$[In(C_2O_4)_3]^{3\ominus}$

M 378.8 (ion)

See μ-(Oxalato-O^1,O^2:O^1,O^2)bis[diaqua(oxalato-$O^1;O^2$)indium], IC-005017.

Tri-H compd.: [22807-41-6].
$C_6H_3InO_{12}$ M 381.9
Microcrystalline solid $+2H_2O$ (H_2O).

Tri-NH_4 salt: White cryst. (H_2O).

Deichman, E.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1964, **9**, 446 (*synth*)
Khantonov, Yu.-Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 460 (*synth, ir*)
Pajakoff, S., *Monatsh. Chem.*, 1969, **100**, 280 (*purif*)
Guru, A.K. *et al*, *Curr. Sci.*, 1976, **45**, 492 (*electrochem*)

IC-005573

$C_6In_2O_{12}$

Indium(*III*) oxalate

Indium ethanedioate (2:3). Ethanedioic acid indium salt. Oxalic acid indium(3+) salt (3:2)

[5066-15-9]

$In_2(C_2O_4)_3$

M 493.6

Crystallises with nH_2O (n = 2-9). White solid. Spar. sol. H_2O.

[38051-36-4]

Diechman, E.N., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1959, **4**, 1207 (*synth, props*)
Kharitonov, Yu.Ya. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 460 (*ir*)
Dutt, N.K. *et al*, *Indian J. Chem., Sect. A*, 1976, **14**, 491; *CA*, 1978, **88**, 202363 (*props*)

IC-005574

$C_6IrN_6^{3\ominus}$

Hexakis(cyano-*C*)iridate(3−), 9CI

Hexacyanoiridate(III)

[19356-47-9]

$[Ir(CN)_6]^{3\ominus}$

M 348.3 (ion)

Forms many salts. Reacts by photosubstitution.

Tri-K salt: [20792-41-0].
$C_6IrK_3N_6$ M 465.6
Commercially available. White cryst. (aq. EtOH). Sol. H_2O.

Di-Cs, Li salt: [42055-52-7].
Cryst. Sol. H_2O. Phase changes at 62, 145°.

Gmelin Handbook Inorg. Chem., Syst. No. 67, 1939, 108; *Suppl.*, 1978, **2**, 181 (*rev, bibl*)
Watt, G.W. *et al*, *J. Inorg. Nucl. Chem.*, 1962, **24**, 1067 (*synth*)
Inoue, H. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 129 (*synth*)
Swanson, B.I. *et al*, *Inorg. Chem.*, 1974, **13**, 313 (*synth, raman, Cs_2Li salt*)
Geoffroy, G. *et al*, *Inorg. Chem.*, 1974, **13**, 430 (*ir, reactions, uv*)
Ryan, R.R. *et al*, *Inorg. Chem.*, 1974, **13**, 1681 (*cryst struct, Cs_2Li salt*)

IC-005575

$C_6K_2Mn_2N_6$

Dipotassium manganese(*II*) hexacyanomanganate(*II*)

[26044-01-9]

$K_2Mn^{II}[Mn^{II}(CN)_6]$

M 344.1

Struct. related to Prussian blue consisting of equal amounts of low spin $Mn^{II}(CN)_6$ and high spin $Mn^{II}(NC)_6$ octahedra. Precipitates from aq. solns. of $K_4Mn(CN)_6$. Oxygen and moisture sensitive dark green solid. Ir ν_{CN} (bridging) 2062 cm^{-1}. μ_{eff} = 4.53μ_B.

Magnuson, W.L. *et al*, *Inorg. Chem.*, 1964, **3**, 88 (*synth*)
Qureschi, A.M. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 2269 (*synth, ir, magnetism, struct, props*)
Rotlevi, E. *et al*, *Can. J. Chem.*, 1970, **48**, 1073 (*synth*)
Sharpe, A.G., *The Chemistry of Cyano Complexes of the Transition Metals*, 1976, 76 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 215 (*rev, bibl*)

IC-005576

$C_6La_2O_{12}$

Lanthanum(*III*) oxalate

Tris(oxalato)dilanthanum(III). *Tris(ethanedioato) lanthanum*(III)

[537-03-1]

$La_2(C_2O_4)_3$

M 541.8

Decahydrate: [14895-97-7].
$C_6H_{20}La_2O_{22}$ M 722.0
Colourless solid. Contains 9 coord. lanthanum. Other hydrates also known.

[6451-21-4, 18901-18-3, 29985-97-5, 70063-08-0, 70063-09-1]

Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth, tga*)
Grebenshchikova, V.I. *et al*, *Radiokhimiya*, 1961, **3**, 486; *Sov. Radiochem.* (*Engl. Transl.*), 1961, **3**, 140.
Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Ollendorff, W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Kartha, V.B. *et al*, *Indian J. Phys., B*, 1980, **54**, 36 (*ir, raman*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)
Hvang, S.-H. *et al*, *J. Crystallogr. Spectrosc. Res.*, 1991, **21**, 127 (*cryst struct*)

IC-005577

$C_6Lu_2O_{12}$

Lutetium(*III*) oxalate

Tris(oxalato)dilutetium(III). *Tris(ethanedioato) dilutetium*(III)

[3426-45-7]

$Lu_2(C_2O_4)_3$

M 613.9

Hexahydrate: [26677-69-0].
$C_6H_{12}Lu_2O_{18}$ M 722.0
Colourless cryst. Presumed 8-coord. by comparison with Yb analogue.

[58176-75-3]

Wendlandt, W.W., *Anal. Chem.*, 1959, **31**, 408 (*tga, dta*)
Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Hansson, E., *Acta Chem. Scand.*, 1973, **27**, 823 (*synth, struct*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*tga, dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

IC-005578

C_6MnNO_5

Pentacarbonyl(cyano-*C*)manganese

[15602-37-6]

$MnCN(CO)_5$

M 221.0

Synth. from $Na[Mn(CO)_5]$ and ICN in THF. Pale-yellow cryst. (Me_2CO). Ir ν_{CN} 2145; ν_{CO} 2075sh, 2055, 1985-1930br cm^{-1}. Dec. *ca* 180°.

Chiswell, B. *et al*, *J. Chem. Soc. A*, 1966, 417 (*synth, ir*)
Fenske, R.F. *et al*, *Inorg. Chem.*, 1971, **10**, 38 (*ir*)

IC-005579

C_6MnNO_5S

Pentacarbonyl(thiocyanato-*S*)manganese(*I*), 10CI

[14874-34-1]

$Mn(SCN)(CO)_5$ (C_{4v})

M 253.0

Golden-yellow cryst. ($CHCl_3$/pet. ether). Sol. CH_2Cl_2, EtOAc, Me_2CO, MeCN, MeOH; spar. sol. PhCl, Et_2O; insol. CCl_4, CS_2. Mp 156° dec. Isom. to *N*-bonded form $Mn(NCS)(CO)_5$ in MeCN. Equil. exists between the two isomers in CH_2Cl_2, $CHCl_3$ or EtOAc. Reacts with donor ligands to give $Mn(SCN)(CO)_4L$ and $Mn(NCS)(CO)_3L_2$, L = R_3N, R_3P, R_3As, R_3Sb.

Farona, M. *et al*, *Inorg. Chem.*, 1965, **4**, 857, 1402 (*synth, ir, props*)

IC-005580

$C_6MnN_3O_3^{2\ominus}$

Tricarbonyltris(cyano-*C*)manganate(2−), 9CI

Tricarbonyltricyanomanganate(I)

$[Mn(CO)_3(CN)_3]^{2\ominus}$

M 217.0 (ion)

fac-Octahedral complex. Reacts with $MeSO_3F$ to give *fac*-$[Mn(CO)_3(CNMe)_3]SO_3F$.

Di-K salt: [14872-97-0].
Synth. from $Mn(NO)(CO)_4$ and KCN in liq. NH_3 or from $MnCl(CO)_5$ and KCN in EtOH at 120° under pressure. Colourless cryst. (NH_3 liq.). Sol. EtOH, liq. NH_3. Ir ν_{CN} 2116vs; ν_{CO} 2014 cm^{-1} (KBr).

Bis-Et_4N salt: [54676-45-8].
Synth. from $MnBr(CO)_5$, KCN and $[Et_4N]Cl$ in MeOH under N_2. Brown solid (Me_2CO/Et_2O). Ir ν_{CN} 2105sh, 2094m; ν_{CO} 2002vs, 1911vs cm^{-1} (CH_2Cl_2).

Brehrens, V.H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **349**, 251; 1969, **365**, 119 (*synth, ir, struct*)
Sawai, T. *et al*, *J. Organomet. Chem.*, 1974, **80**, 91 (*synth, ir, reactions*)
Compr. Organomet. Chem., Pergamon, Oxford, 1982, **4**, 59 (*rev, bibl*)

IC-005581

$C_6MnN_4O_2^{3\ominus}$

Dicarbonyltetrakis(cyano-*C*)manganate(3−)

Dicarbonyltetracyanomanganate(I)(3−)

$[(OC)_2Mn(CN)_4]^{3\ominus}$

M 215.0 (ion)

cis-Octahedral.

Tri-K salt: [14872-98-1].
Synth. from $Mn_2(CO)_{10}$ and KCN in liq. NH_3 at 120°. Colourless needles (NH_3 liq.). Ir ν_{CN} 2178vs, 2092s, 2075m, 2049s; ν_{CO} 1917vs, 1833vs cm^{-1} (KBr).

Behrens, H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **349**, 251 (*synth, ir*)

IC-005582

$C_6MnN_6^{5\ominus}$

Hexakis(cyano-*C*)manganate(5−), 11CI

Hexacyanomanganate(I)(5−)

[19567-57-8]

$[Mn(CN)_6]^{5\ominus}$ (O_h)

M 211.0 (ion)

Synth. by reducing $[Mn(CN)_6]^{4\ominus}$ with Na or K amalgams, Al or Mn powder or electrolytically in absence of O_2. Yellow aq. solns. undergo oxidn.: $[Mn(CN)_6]^{5\ominus} \rightleftharpoons [Mn(CN)_6]^{4\ominus}$ reversible. E° for $Mn^I \rightarrow Mn^{II} + e^\ominus$ in 1.5*M* NaOH is −1.06V at 25°. Diamagnetic, low spin d^6 anion.

Penta-Na salt:
$C_6MnN_6Na_5$ M 325.9
Colourless cryst., readily oxidised in moist air; dec. in dry CO_2. Liberates H_2 from hot H_2O.

Penta-K salt: [20558-43-4].
$C_6K_5MnN_6$ M 406.5
Colourless cryst., readily oxidised in moist air; dec. in dry CO_2.

Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1970, 858 (*ir, raman*)
Krasser, W. *et al*, *Z. Naturforsch., A*, 1972, **27**, 1193 (*ir, raman*)
Griffith, W.P., *Coord. Chem. Rev.*, 1975, **17**, 177 (*rev*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1594 (*synth*)
Sharpe, A.G., *Chemistry of the Cyano Complexes of the Transition Metals*, Academic Press, London, 1976, 76 (*rev, bibl*)
Hauck, J., *Inorg. Nucl. Chem. Lett.*, 1976, **12**, 893 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 197 (*rev, bibl*)

IC-005583

$C_6MnN_6^{4\ominus}$

Hexakis(cyano-*C*)manganate(*II*)(4−), 11CI

Hexacyanomanganate(II)(4−)

[14931-64-7]

$[Mn(CN)_6]^{4\ominus}$ (O_h)

M 211.0 (ion)

Synth. by treating $Mn(OAc)_2$ or $MnCO_3$ with excess aq. $CN^\ominus$ under rigorous exclusion of O_2. $t_{\frac{1}{2}}$ $CN^\ominus$ exchange *ca.* 5 min. at pH 11.8. Aq. solns. are yellow and readily lose $CN^\ominus$ unless excess $CN^\ominus$ concs. at 1.5*M* present. They contain several Mn spp. and dec., depositing green insol. products which appear to contain the ion $[Mn^{II}[Mn^{II}(CN)_6]]^{2\ominus}$. Low spin d^6 anion 10dq 30,000 cm^{-1}. $Mn(CN)_6^{3\ominus}/Mn(CN)_6^{4\ominus}$ couple 0.24V.

Tetra-Na salt, decahydrate: [33913-99-4].
Synth. from $MnCO_3$ and NaCN. Yellow cryst. (H_2O); unstable in air. Mn—C 195.3 pm.

Tetra-K salt, 11CI: [14874-32-9].
$C_6K_4MnN_6$ M 367.4
Synth. by heating the trihydrate at 100° *in vacuo*. Grey-violet.

Tetra-K salt, trihydrate: [14323-52-5].
Synth. by action of excess KCN on $MnCO_3$. Blue-purple cryst. (aq. KCN >1.5*M*), oxygen sensitive, efflorescent. μ_{eff} = 2.18μ_B (300K). Blue colour suggests presence of some Mn^{III} or Mn^{IV} and electron transfer band. Dissolves in aq. KCN to give yellow solns.

Di-K, Mn(II) *salt:* see *Dipotassium manganese*(II) *hexacyanomanganate*(II), *IC-005575*
[14023-98-4]

Figgis, B.N., *Trans. Faraday Soc.*, 1961, **57**, 204 (*magnetism*)
Magnuson, W.L. *et al*, *Inorg. Chem.*, 1964, **3**, 88 (*synth, props*)
Ratlevi, E. *et al*, *Can. J. Chem.*, 1970, **48**, 1073 (*esr*)
Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1970, 858 (*raman*)
McCarthy, A.E., *J. Chem. Soc. A*, 1970, 1379 (*ir, uv*)

Tulberg, A. *et al, Acta Chem. Scand., Ser. A*, 1974, **28**, 551 (*cryst struct*)
Griffith, W.P., *Coord. Chem. Rev.*, 1975, **17**, 177 (*rev, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1594 (*synth*)
Sharpe, A.G., *Chemistry of the Cyano Complexes of the Transition Metals*, Academic Press, London, 1976, 76 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 202 (*rev, bibl*)

IC-005584

$C_6MnN_6^{3\ominus}$

Hexakis(cyano-*C*)manganate(3−), 11CI

Hexacyanomanganate(III)(*3*−)

[14931-63-6]

$[Mn(CN)_6]^{3\ominus}$ (O_h)

M 211.0 (ion)

Early work on the physical properties of $[Mn(CN)_6]^{3\ominus}$ is in doubt since products may have been contaminated with $[(NC)_5Mn—O—Mn(CN)_5]^{6\ominus}$. Low spin d^4 octahedral complex anion. $[Mn(CN)_6]^{3\ominus} + e^{\ominus} \rightarrow [Mn(CN)_6]^{4\ominus}$; E° −0.24 V.

Tri-Na salt: [14023-97-3].
Synth. from so-called $Mn(OAc)_3.2H_2O$ and NaCN. Red cryst. + $3H_2O$.

Tri-K salt: [14023-90-6].
Synth. from freshly prepd. $MnCO_3$ and aq. KCN followed by oxidn. of the blue soln. of $K_4Mn(CN)_6$ with 3% H_2O_2. Air-stable dark red-brown needles (10% KCN/EtOH). $\mu_{eff} = 3.50\mu_B$ (r.t.). Undiluted salt shows no esr signal between 12-290K. Mn—C_{av} 198 pm. Dec. by H_2O to give hydrated Mn_2O_3.

Di-Cs, Li salt: [37164-28-6].
Synth. from stoichiometric amounts of $Li_3[Mn(CN)_6]$ and $Cs_3[Mn(CN)_6]$ in H_2O. Red cryst. (H_2O).

Tris-Et$_4$N salt: [67265-39-8].
Synth. from Et_4NClO_4 and $K_3Mn[(CN)_6]$ in MeOH.

Cooke, A.H. *et al, Proc. Phys. Soc. A (London)*, 1955, **68**, 32 (*magnetism*)
Griffith, W.P. *et al, J. Chem. Soc. A*, 1970, 858 (*raman*)
Bailey, R.A. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 2668 (*uv*)
Swanson, B.I. *et al, Inorg. Chem.*, 1973, **12**, 283 (*cryst struct, synth*)
Gupta, M.P. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 656 (*cryst struct*)
Ryan, R.R. *et al, Inorg. Chem.*, 1974, **13**, 1681 (*cryst struct*)
Griffith, W.P., *Coord. Chem. Rev.*, 1975, **17**, 177 (*rev, bibl*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1594 (*synth*)
Trageser, G. *et al, Inorg. Nucl. Chem. Lett.*, 1978, **14**, 65 (*synth, ir*)
Gritzner, G. *et al, J. Electroanal. Chem. Interfacial Electrochem.*, 1978, **90**, 203 (*synth, uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 218 (*rev, bibl*)

$C_6MnN_6^{2\ominus}$

IC-005585

Hexakis(cyano-*C*)manganate(*IV*)(2−), 11CI

Hexacyanomanganate(IV)(*2*−)

[66735-85-1]

$[Mn(CN)_6]^{2\ominus}$ (O_h)

M 211.0 (ion)

Di-K salt: [28299-84-5].
Synth. by oxidising corresp. Mn(*III*) salt in DMF with NOCl. Canary yellow solid. $\mu_{eff} = 3.94\mu_B$, high spin d^3 sp.

Mn(II) *salt:* [74506-85-7]. *Manganese*(II) *hexacyanomanganate*(IV). *Manganese cyanide* ($Mn(CN)_3$) (*incorr.*)

$C_6Mn_2N_6$ M 265.9
Precipitates from aq. solns. of $[Mn(CN)_6]^{3\ominus}$ or by hydrol. of $Na_3Mn(CN)_6.3H_2O$ with 20% $HClO_4$. Violet-brown solid + H_2O; uncertain degree of hydration. Previously formulated as $Mn(CN)_3.nH_2O$. Zn(*II*) and Cd(*II*) salts also known. Mixed valence compd. containing six fold N-coordinated Mn(*II*) and $Mn(CN)_6^{2\ominus}$ in a fcc lattice.

Fowler, J.R. *et al, Inorg. Chem.*, 1970, **9**, 1005 (*synth, ir, magnetism*)
Trageser, G. *et al, Z. Anorg. Allg. Chem.*, 1976, **420**, 273 (*struct, uv-vis, ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 248 (*rev, bibl*)
Klenze, R. *et al, J. Chem. Phys.*, 1980, **72**, 5819 (*synth, magnetism, powder struct, uv, ir*)

$C_6MnN_6S_6^{4\ominus}$

IC-005586

Hexakis(thiocyanato-*N*)manganate(*II*)(4−), 9CI

Hexaisothiocyanatomanganate(II)(*4*−)

[21790-84-1]

$[Mn(NCS)_6]^{4\ominus}$ (O_h)

M 403.4 (ion)

Synth. from $Mn^{2\oplus}$ and KSCN in MeOH.

Tetrakis-Me$_4$N salt: Synth. from $Mn(NO_3)_2.4H_2O$ and $[Me_4N]SCN$ in MeOH. Mp 280° dec.

Tetrakis-Et$_4$N salt: Synth. from $MnCl_2$, KSCN and $[Et_4N]Br$ in EtOH. Colourless cryst. $\mu_{eff} = 5.93\mu_B$ (295K).

Salzmann, J.J. *et al, Inorg. Chim. Acta*, 1969, **3**, 207 (*magnetism*)
Schmidtke, H.H. *et al, Z. Naturforsch., A*, 1969, **24**, 126 (*synth*)
Clark, R.J.H. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 323 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 287 (*rev, bibl*)

$C_6MnN_6Se_6^{4\ominus}$

IC-005587

Hexakis(selenocyanato-*N*)manganate(*II*)(4−)

Hexaisoselenocyanatomanganate(*4*−)

$[Mn(NCSe)_6]^{4\ominus}$ (O_h)

M 684.8 (ion)

Tetrakis-Me$_4$N salt: [10210-87-4].
Synth. from $MnCl_2.4H_2O$ and $Me_4N[SeCN]$ in EtOH. Pink cryst. (MeOH). Mp 279°. $\mu_{eff} = 5.86\mu_B$ (295 K).

Forster, D. *et al, Inorg. Chem.*, 1965, **4**, 1712 (*synth, ir*)
Burmeister, J.L. *et al, Inorg. Chem.*, 1966, **5**, 1113 (*ir*)
Salzmann, J.J. *et al, Inorg. Chim. Acta*, 1969, **3**, 207 (*magnetism*)
Schmidtke, H.H. *et al, Z. Naturforsch., A*, 1969, **24**, 126 (*props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 293 (*rev, bibl*)

$C_6MnO_6^{\oplus}$

IC-005588

Hexacarbonylmanganese(1+), 9CI

Manganesehexacarbonyl(*1*+)

[21331-06-6]

$[Mn(CO)_6]^{\oplus}$ (O_h)

M 223.0 (ion)

Synth. from $MnCl(CO)_5$, $AlCl_3$ and CO at 250 atm or from $HMn(CO)_5$, HO_3SCF_3 and CO at 0.9 atm.

Tetrafluoroborate: [15557-71-8].
White solid.

Fischer, E.O. *et al, Chem. Ber.*, 1962, **95**, 249 (*synth, props*)
Kruck, T. *et al, Chem. Ber.*, 1964, **97**, 1693 (*synth*)
Beach, N.A. *et al, J. Am. Chem. Soc.*, 1968, **90**, 5713 (*synth, uv*)

DeKock, R.L. *et al, Inorg. Chem.*, 1971, **10**, 38 (*struct*)
Darensbourg, D.J. *et al, J. Am. Chem. Soc.*, 1977, **99**, 4726 (*props*)
Trogler, W.C., *J. Am. Chem. Soc.*, 1979, **101**, 6459 (*synth*)

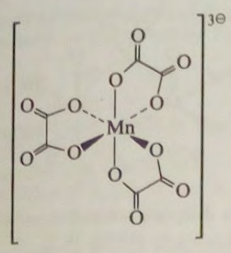
IC-005589

$C_6MnO_{12}^{3\ominus}$

Tris(oxalato)manganate(*III*)(3−)

Tris[ethanedioato(2−)-O,O′]manganate(III)(*3*−), *11CI*

[16961-54-9]



M 318.9 (ion)

Octahedral with Jahn-Teller distortion. Compds. and their aq. solns. dec. easily, especially in light or when heated. Readily hydrol. to $[Mn(C_2O_4)_2(H_2O)_2]^{2\ominus}$.

Tri-K salt: [21647-79-0].
Synth. by treating $KMnO_4$ with hot aq. oxalic acid followed by addition of K_2CO_3. Deep red-purple cryst. + $3H_2O$. Sol. H_2O; sl. sol. MeOH; insol. EtOH, Me_2CO, Et_2O. Dec. at *ca.* 80° to give $K_2[Mn(C_2O_4)_2]$.

Cartledge, G.H. *et al, J. Am. Chem. Soc.*, 1936, **58**, 2061 (*synth, props*)
Furlani, C. *et al, Ann. Chim. (Rome)*, 1958, **48**, 286 (*magnetism*)
Bancroft, G.M. *et al, Inorg. Nucl. Chem. Lett.*, 1970, **6**, 403 (*props*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1592 (*synth*)
Lis, T. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 1938 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 108 (*rev, bibl*)

$C_6Mn_2N_2O_8^{2\ominus}$

IC-005590

Hexacarbonyldinitrosyldimanganate(2−)

$[(ON)(OC)_3Mn—Mn(CO)_3(NO)]^{2\ominus}$

M 337.9 (ion)

Bis[bis(triphenylphosphine)iminium] salt: [84928-63-2].
Synth. from $K_2[Mn(NO)(CO)_3]$ and $Mn(NO)(CO)_4$ in THF followed by addition of $[(Ph_3P)_2N]Cl$. Air-stable bright-orange cryst. Ir ν_{CO} 1970m, 1890s, 1860s; ν_{NO} 1650m, 1610s cm^{-1} (THF).

Chen, Y.-S. *et al, J. Am. Chem. Soc.*, 1983, **105**, 1689 (*synth, ir, pmr*)

$C_6Mn_2O_{12}^{2\ominus}$

IC-005591

Tris(oxalato)dimanganate(*II*)(2−)

$[Mn_2(C_2O_4)_3]^{2\ominus}$

M 373.9 (ion)

Di-Cs salt: Synth. from $Cs_2C_2O_4$ and MnC_2O_4 in H_2O. Cryst. + $3H_2O$. Polymeric struct. with $MnO_5(H_2O)$ octahedra.

Siems, H. *et al, Z. Anorg. Allg. Chem.*, 1972, **393**, 97 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 106 (*rev, bibl*)

$C_6MoNO_5^{\ominus}$

IC-005592

Pentacarbonyl(cyano-*C*)molybdate(1−), 8CI

$[MoCN(CO)_5]^{\ominus}$

M 262.0 (ion)

Bis(triphenylphosphine)iminium salt: [39048-39-0].
White cryst.

King, R.B., *Inorg. Chem.*, 1967, **6**, 25 (*synth, props*)
Ruff, J.K. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 215.

$C_6MoN_6^{4\ominus}$

IC-005593

Hexakis(cyano-*C*)molybdate(*II*)(4−), 11CI

[87698-69-9]

$[Mo(CN)_6]^{4\ominus}$

M 252.0 (ion)

Struct. not descr.

Tetra-K salt: [14023-94-0].
Synth. from $K_4[Mo(CN)_8]$ and H_2. Green or black solid, green in aq. soln.; aq. soln. strong reducing agent. $\mu_{eff} = 1.13\mu_B$.

Yoo, J.S. *et al, Inorg. Chem.*, 1965, **4**, 365 (*synth, ir*)
Zubritskaya, D.I. *et al, Koord. Khim.*, 1983, **9**, 1073.

$C_6MoN_6S_6^{3\ominus}$

IC-005594

Hexakis(thiocyanato-*N*)molybdate(*III*)(3−)

Hexakis(isothiocyanato)molybdate(*3*−), *8CI*.
Hexaisothiocyanatomolybdate(III)

$[Mo(NCS)_6]^{3\ominus}$ (O_h)

M 444.4 (ion)

Octahedrally coordinated Mo. Mo—N_{av} 208.8 pm.

Tri-K salt: [19498-23-8].
Transparent yellow cryst. + $1H_2O$ + 1AcOH (2*M* AcOH).

Knox, J.R. *et al, Inorg. Chem.*, 1968, **7**, 84 (*cryst struct*)

C_6MoO_6

IC-005595

Hexacarbonylmolybdenum

Molybdenum hexacarbonyl. Molybdenum carbonyl (*Mo*(*CO*)$_6$), *10CI*

[13939-06-5]

$Mo(CO)_6$

M 264.0

Catalyst for allylic alkylation reactions. Important starting material (commercially available). Colourless, odourless, air-stable, diamagnetic solid. Sol. org. solvs.

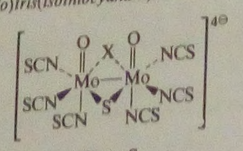
Junk, G.A. *et al, Z. Naturforsch., B*, 1968, **23**, 1 (*ms*)
Jones, L.H. *et al, Inorg. Chem.*, 1969, **11**, 2349 (*ir*)
Mann, B.E., *J. Chem. Soc., Dalton Trans.*, 1973, 2012 (*nmr*)
Lloyd, D.R. *et al, J. Chem. Soc., Faraday Trans. 2*, 1973, **69**, 1659 (*pe*)
Hagan, A.P. *et al, Inorg. Chem.*, 1978, **17**, 1369 (*synth*)
Michels, G.D. *et al, Inorg. Chem.*, 1980, **19**, 479.
Trost, B.M. *et al, J. Am. Chem. Soc.*, 1987, **109**, 1469 (*use*)
Perez, D. *et al, J. Org. Chem.*, 1987, **52**, 5570 (*use*)
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 1852.

IC-005596

$C_6Mo_2N_6O_2S_8^{4\ominus}$

Dioxohexakis(thiocyanato-*N*)di-μ-thioxodimolybdate(4−), 11CI

Bis[(μ_2-*sulfido*)*tris*(*isothiocyanato*)*oxomolybdate*(V)]



X = S

M 636.5 (ion)

Each Mo(*V*) ion has a distorted octahedral coordination. Interatomic distances: Mo—Mo 282.7, Mo=O 168.3, Mo—S 230.1, 231.3, Mo—N 217.6, 218.3, 226.9 pm.

Tetrakis-pyridinium salt: [88430-21-1].
Red prisms.

Shibahara, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 2945 (*cryst struct, synth*)

IC-005597

$C_6Mo_2N_6O_3S_7^{4\ominus}$

μ-Oxodioxohexakis(thiocyanato-*N*)-μ-thioxodimolybdate(4−), 11CI

μ_2-*Oxo*-μ_2-*sulfidobis*[*tris*(*isothiocyanato*)*oxomolybdate*(V)]

As Dioxohexakis(thiocyanato-*N*)di-μ-thioxodimolybdate(4−), IC-005596 with

X = O

M 620.4 (ion)

Each Mo(*V*) ion is in a distorted octahedral environment. Interatomic distances: Mo—Mo 268.2, Mo=O 166.9, Mo—O 195.0, Mo—S 230.8, Mo—N 217.0, 217.0, 227.0 pm.

Tetrakis-pyridinium salt: [88430-23-3].
Thin red plates + $2H_2O$.

Shibahara, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 2945 (*cryst struct, synth*)

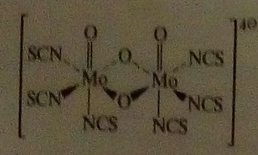
IC-005598

$C_6Mo_3N_6O_4S_6^{4\ominus}$

Di-μ-oxodioxohexakis(thiocyanato-*N*)dimolybdate(*V*)(4−), 11CI, 10CI, 9CI

Hexa(*isothiocyanato*)*di*-μ-*oxodioxodimolybdate*(V). *Di*-μ-*oxobis*[*oxotris*(*isothiocyanato*)*molybdate*(V)]

[103591-07-7]



M 604.3 (ion)

6-Coord. Mo in approx. octahedral config., Mo—Mo 258.2 pm.

Tetrakis-pyridinium salt: [52581-99-4].
Red cryst. Sol. Me_2CO, hot EtOH. Mp 181°. μ_{eff} = 0.59μ_B (293K).

[22323-42-8, 73752-47-3, 74310-35-3]

Mitchell, P.C.H. *et al*, *J. Chem. Soc.*, 1962, 4570 (*synth, props*)
Jezowska-Trzebiatowska, B. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1977, **22**, 1590 (*synth, cryst struct*)
Kamenar, B. *et al*, *Z. Kristallogr.*, 1979, **150**, 327 (*cryst struct*)
Shibahara, T. *et al*, *Inorg. Chim. Acta*, 1983, **76**, L315

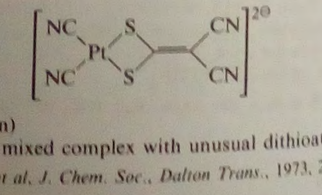
Chakravorti, M.C. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1985, **15**, 1 (*reactions*)
Yao, Q. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 5364.

$C_6Mo_2N_6O_7S_7^{4\ominus}$

IC-005599

μ-Oxodioxo[μ-[sulfato(2−)-*O,O'*]]hexakis(thiocyanato-*N*)dimolybdate(*V*)(4−), 11CI

μ_2-*Oxo*-μ_2-*sulfatobis*[*oxotriisothiocyanatomolybdate*(V)]



M 684.4 (ion)

Mo atoms have distorted octahedral geometry.

Tetrakis-pyridinium salt: [97589-38-3].
Cryst.

Yang Rongsheng, *et al*, *Jiegou Huaxue*, 1984, **3**, 101 (*cryst struct*)

$C_6NO_5W^{\ominus}$

IC-005600

Pentacarbonyl(cyano-*C*)tungstate(1−), 10CI

[68927-82-2]

$[(OC)_5WCN]^{\ominus}$

M 349.9 (ion)

Et_4N salt: [77827-07-7].
White cryst. Sol. H_2O.

Bis(*triphenylphosphine*)*iminium salt:* [22043-88-5].
White cryst.

King, R.B., *Inorg. Chem.*, 1967, **6**, 25.
Ruff, J.K. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1971, **1**, 215 (*synth*)
Fehlhammer, W.P. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1979, **18**, 75 (*props*)
Angelici, R.J. *et al*, *Inorg. Chem.*, 1981, **20**, 2977 (*synth*)

$C_6N_4PtS_2^{2\ominus}$

IC-005601

Bis(cyano)[(dimercaptomethylene)propanedinitrilo]platinate(2−), 9CI

[51405-03-9]

M 387.3 (ion)

Example of mixed complex with unusual dithioate ligand.

Hynes, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2280.

$C_6N_6NbS_6^{2\ominus}$

IC-005602

Hexakis(thiocyanato-*N*)niobate(*IV*)(2−)

Hexakis(*isothiocyanato*)*niobate*(IV)(*2*−), *8CI*.
Hexaisothiocyanatoniobate(IV)(*2*−)

$[Nb(NCS)_6]^{2\ominus}$ (O_h)

M 441.4 (ion)

Di-K salt: [26032-41-7].
Synth. by dissolving $NbCl_5$ in MeCN then adding KNCS. Cryst. ($MeCN/CH_2Cl_2$). Sol. MeCN.

Knox, G.F. *et al*, *Inorg. Chem.*, 1969, **8**, 1401 (*synth, ir, uv-vis*)

IC-005603

$C_6N_6NbS_6^{\ominus}$

Hexakis(thiocyanato-*N*)niobate(*V*)(1−), 10CI

Hexakis(*isothiocyanato*)*niobate*(V)(*1*−), *8CI*.
Hexaisothiocyanatoniobate(V)(*1*−)

[16919-15-6]

$[Nb(NCS)_6]^{\ominus}$ (O_h)

M 441.4 (ion)

In soln., a variety of combinations of *S*- and *N*-bonded thiocyanates have been observed by ^{93}Nb nmr. Sol. MeCN.

K salt: [17979-22-5].
$C_6KN_6NbS_6$ M 480.5
Synth. from $NbCl_5$ and KNCS in MeCN. Lustrous blue solid (CH_2Cl_2). Mp > 250°.

Tetrabutylammonium salt: [26032-39-3].
Obt. by metathesis of K salt in MeCN. Lustrous blue solid. Mp 122°.

Ph_4As salt: [16921-87-2].
Obt. by metathesis of K salt. Lustrous blue solid. Mp 222°.

Brown, T.M. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 5296 (*synth, derivs*)
Knox, G.F. *et al*, *Inorg. Chem.*, 1969, **8**, 1401 (*synth, ir, derivs*)
Inorg. Synth., 1971, **13**, 226 (*synth, K salt*)
Kidd, R.G. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4759 (*Nb-93 nmr*)

$C_6N_6NiS_6^{4\ominus}$

IC-005604

Hexakis(thiocyanato-*N*)nickelate(*II*)(4−), 9CI

Hexakis(*isothiocyanato*)*nickelate*(II)(*4*−).
Hexathiocyanatonickelate(II)(*4*−)

[21780-87-0]

$[Ni(NCS)_6]^{4\ominus}$

M 407.1 (ion)

N atoms bonded to Ni. Paramagnetic.

Tetra-K salt: [19341-43-6].
$C_6K_4N_6NiS_6$ M 563.5
Blue-green solid.

Norbury, A.H., *Adv. Inorg. Chem. Radiochem.*, 1975, **17**, 309.

$C_6N_6NiSe_6^{4\ominus}$

IC-005605

Hexakis(selenocyanato-*N*)nickelate(*II*)(4−), 9CI

Hexakis(*isoselenocyanato*)*nickelate*(II)(*4*−).
Hexaselenocyanatonickelate(II)(*4*−)

[23195-19-9]

$[Ni(NCSe)_6]^{4\ominus}$

M 688.5 (ion)

N atoms bonded to Ni. Paramagnetic. Best isol. as $R_4N^{\oplus}$ salts.

Tetrakis-Et_4N salt: [10478-60-1].
Blue-green solid.

Norbury, A.H., *Adv. Inorg. Chem. Radiochem.*, 1975, **17**, 313.

$C_6N_6Ni_2^{4\ominus}$

IC-005606

Hexakis(cyano-*C*)dinickelate(4−), 10CI

Hexakiscyanodickelate(*4*−), *9CI*. *Hexacyanodinickelate*(II)(*4*−)

$[(N{\equiv}C)_3Ni{-}Ni(C{\equiv}N)_3]^{4\ominus}$

M 273.4 (ion)

The two almost planar $Ni(CN)_3$ units are at an angle to one another.

Tetra-K salt: [12387-13-2]. *Belluci's salt*
$C_6K_4N_6Ni_2$ M 429.8
Synth. from $K_2Ni(CN)_4$ and Na/liq. NH_3, Na/Hg or H_2. Catalyses oligomerisation of disubstituted acetylenes. Air-sensitive, deep red solid (EtOH), aq. soln. dec. on standing, diamagnetic. Sol. H_2O. Dec. slowly in air to yellow solid.
Tetra-Rb salt: [34054-84-7].
Dark violet cryst.

[40810-33-1]

Eastes, J.W. *et al*, *J. Am. Chem. Soc.*, 1942, **64**, 1187 (*synth, props, deriv*)
Inorg. Synth., 1957, **5**, 197 (*synth*)
Griffith, W.P. *et al*, *J. Inorg. Nucl. Chem.*, 1958, **7**, 295 (*props, ir, deriv*)
Yoo, J.S. *et al*, *Inorg. Chem.*, 1965, **4**, 365 (*synth, props, deriv*)
Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1969, 834 (*ir*)
Jarchow, O., *Z. Anorg. Allg. Chem.*, 1971, **383**, 40 (*cryst struct, Rb salt*)
Jarchow, O., *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1972, **136**, 122 (*cryst struct, K salt*)
Matienzo, J. *et al*, *Inorg. Chem.*, 1973, **12**, 2762 (*pe, K salt*)
de Haas, K.S. *et al*, *Inorg. Chim. Acta*, 1977, **24**, 269 (*ir*)

$C_6N_6O_3Ru^{3\ominus}$

IC-005607

Bis(cyanato-*N*)tetrakis(cyano-*C*)oxoruthenate(*V*)(3−), 9CI

Tetracyanobis(*isocyanato*)*oxoruthenate*(V)

$[O{=}Ru(CN)_4(NCO)_2]^{3\ominus}$

M 305.1 (ion)

Struct. unknown.

Tri-Cs salt: [42720-51-4].
$C_6Cs_3N_6O_3Ru$ M 703.8
Prepd. by treating RuO_4 with aq. NaCN (0°) in the presence of $Cs^{\oplus}$. Green salt. μ_{eff} = 3.0μ_B; Ir $\nu_{Ru=O}$ 787 cm^{-1}.

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)

$C_6N_6Os^{4\ominus}$

IC-005608

Hexakis(cyano-*C*)osmate(*II*)(4−), 9CI

Hexacyanoosmate(II)(*4*−)

[19356-45-7]

$[Os(CN)_6]^{4\ominus}$ (O_h)

M 346.3 (ion)

Many salts known.

Tetra-Na salt: [16997-02-7].
Synth. by metathesis of K salt. White needles (EtOH).
Tetra-K salt: [20740-36-7].
Synth. from K_2OsO_4 and KCN. Air-sensitive square white plates. Hydrol. in H_2O.
Di-Cu salt: [41898-56-0].
Synth. from $K_2[Os(CN)_6]$ and $CuSO_4$ in dil. H_2SO_4. Flaky yellow brown solid + xH_2O.
Di-Ni salt: [36535-39-4].
Analogous synth. to di-Cu salt. Grey blue flaky solid. Acid-stable, freshly prepd. salts react with alkali.

[14323-54-7]

Waku, S. *et al*, *J. Phys. Soc. Jpn.*, 1960, **15**, 1185 (*cryst struct*)
Robin, M.B. *et al*, *Inorg. Chem.*, 1962, **1**, 337 (*uv*)
Masuno, K. *et al*, *Nippon Kagaku Zasshi* (*Jpn. J. Chem.*), 1962, **83**, 116 (*uv*)
Bramley, R. *et al*, *J. Chem. Soc. A*, 1967, 861 (*synth, nmr, ir*)
White, D.L. *et al*, *Biochim. Biophys. Acta*, 1976, **436**, 577 (*pe*)
Pesek, J.J. *et al*, *Inorg. Chem.*, 1979, **18**, 924 (*cmr*)

IC-005609

$C_6N_6Os^{3\ominus}$

Hexakis(cyano-*C*)osmate(*III*)(3−), 9CI
Hexacyanoosmate(III)(*3*−)
[45046-99-9]

$[Os(CN)_6]^{3\ominus}$

M 346.3 (ion)
Easily reduced to $[Os(CN)_6]^{4\ominus}$. Obt. by electrochemical oxidation of $[Os(CN)_6]^{4\ominus}$.
Tri-K salt: [38192-69-7].
Tris-tetrabutylammonium salt: [20792-37-4].
Yellow plates (CH_2Cl_2/hexane). $\mu_{eff} = 2.12\mu_B$ (296K).

Meites, L., *J. Am. Chem. Soc.*, 1957, **79**, 4631 (*props, use*)
Alexander, J.J., *J. Am. Chem. Soc.*, 1968, **90**, 4260 (*synth, ir, uv, Bu_4N salt*)
Juris, A. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 1047 (*photochem*)
Opekar, F. *et al*, *J. Electroanal. Chem. Interfacial Electrochem.*, 1976, **71**, 120 (*synth*)

IC-005610

$C_6N_6OsS_6^{3\ominus}$

Hexakis(thiocyanato)osmate(*III*)(3−)
Hexathiocyanatoosmate(III)

$[Os(NCS)_n(SCN)_{6-n}]^{3\ominus}$ (O_h)

M 538.7 (ion)
Forms a series of 10 isomers of formula $[Os(NCS)_n(SCN)_{6-n}]^{3\ominus}$. *N*-bonded isomers are thermodynamically more stable. The pure isomers are obt. by ion exchange chromatography on diethylaminoethylcellulose.

Hexakis-thiocyanato-S-form [48072-45-3]
*Hexakis(thiocyanato-*S*)osmate*(III)(*3*−)
Tris-tetrabutylammonium salt: [19584-47-5].
Raspberry red.

Mono-thiocyanato-N-form [72124-85-7]
(*Thiocyanato-*N*)pentakis(thiocyanato-*S*)osmate*(*3*−)
Tris-tetrabutylammonium salt: [72124-86-8].
Yellowish-red. Mp 200-205°.

Bis-thiocyanato-N-form [61202-53-7]
*Bis(thiocyanato-*N*)tetrakis(thiocyanato-*S*)osmate*(*3*−)
Exists as *cis* and *trans* stereoisomers. Synth. from $K_2[OsCl_6]$ and aq. KSCN. at reflux temp. (*trans*-form), or at 60° *cis*-form. Obt. as a majority of one isomer and separated by ion exchange chromatography.
Tris-tetrabutylammonium salt: [61202-54-8].
Red orange. Mp 175-180°. Props. for *cis* and *trans*-forms not separately reported.

Tris-thiocyanato-N-form [61202-55-9]
*Tris(thiocyanato-*N*)tris(thiocyanato-*S*)osmate*(*3*−)
Exists as *mer* and *fac*-stereoisomers. Synth. from $K_2[OsCl_6]$ and aq. KSCN. at reflux temp. (*mer*-form) or at 60° (*fac*-form). Obt. as mixtures with majority of one isomer, separated by ion exchange chromatography.
Tris-tetrabutylammonium salt: [61202-56-0].
Mp 155-160°. Props. for *mer* and *fac*-forms not separately reported.

Tetrakis-thiocyanato-N-form [61202-57-1]
*Tetrakis(thiocyanato-*N*)bis(thiocyanato-*S*)osmate*(*3*−)
Exists as *cis* and *trans*-forms. Synth. from $K_2[OsCl_6]$ and aq. KSCN at reflux temp. (*trans*-form) or at 60° (*cis*-form). Obt. as mixtures with majority of one isomer, separated by ion exchange chromatography.
Tris-tetrabutylammonium salt: [61202-58-2].
Yellow orange solid. Mp 160-165°. Props. for *cis* and *trans*-forms not separately reported.

Pentakis-thiocyanato-N-form
*Pentakis(thiocyanato-*N*)mono(thiocyanato-*S*)osmate*(*3*−)
Tris-tetrabutylammonium salt: Orange yellow. Mp 175-177°.

Hexakis-thiocyanato-N-form [45229-50-3]
*Hexakis(thiocyanato-*N*)osmate*(*3*−)
Tris-tetrabutylammonium salt: [18041-93-5].
Yellow solid. Mp 185°.

[72124-87-9, 72124-88-0, 75365-17-2, 75365-18-3, 75365-19-4, 75365-20-7, 75365-21-8, 75365-22-9, 75365-23-0, 75365-24-1, 75365-25-2, 75365-26-3, 75597-84-1, 75597-85-2]

Schmidtke, H.H. *et al*, *Helv. Chim. Acta*, 1967, **50**, 1631.
Salzmann, J.J. *et al*, *Inorg. Chim. Acta*, 1969, **3**, 207.
Bailey, R.A. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 3206.
Schwerdteger, *et al*, *Angew. Chem., Int. Ed. Engl.*, 1977, **16**, 108 (*ir, raman*)
Rabe, P. *et al*, *Z. Naturforsch., A*, 1979, **34**, 1528 (*struct*)
Preetz, W. *et al*, *Z. Naturforsch., B*, 1979, **34**, 1243 (*ir, raman, synth, uv-vis*)
Peters, G. *et al*, *Z. Naturforsch., B*, 1980, **35**, 994 (*synth*)
Buetje, K. *et al*, *Z. Naturforsch., B*, 1988, **43**, 371, 382 (*ir, raman*)

IC-005611

$C_6N_6Pd^{2\ominus}$

Hexakis(cyano-*C*)palladate(2−), 9CI
Hexacyanopalladate(IV)
[20740-37-8]

$[Pd(CN)_6]^{2\ominus}$

M 262.5 (ion)
Di-K salt: [25737-15-9].
$C_6K_2N_6Pd$ M 340.7
Prepd. by reaction of K_2PdCl_6 with KCN in aq. soln. in the presence of $K_2S_2O_8$. Colourless prisms (H_2O). Dec. slowly above 160°. Mod. sol. H_2O; sl. sol. EtOH; insol. Et_2O.

[30142-14-4, 30142-16-6, 30142-17-7, 30142-18-8, 30233-32-0, 30233-33-1, 30233-34-2, 32492-30-1, 41876-14-6]

Siebert, H. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1969, **8**, 600 (*synth*)
Siebert, H. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **378**, 160 (*synth, uv, ir, raman*)
Siebert, H. *et al*, *Z. Naturforsch., B*, 1972, **27**, 865 (*synth, ir*)
Buser, H.-J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2473 (*cryst struct*)
Pesek, J.J. *et al*, *Inorg. Chem.*, 1979, **18**, 924 (*cmr*)

IC-005612

$C_6N_6PrS_6^{3\ominus}$

Hexakis(thiocyanato-*N*)praseodymate(3−)
Hexaisothiocyanatopraseodymate(*3*−)

$[Pr(NCS)_6]^{3\ominus}$ (O_h)

M 489.4 (ion)
Tris-tetrabutylammonium salt: [26395-50-6].
Pale yellow-green cryst. (EtOH/1-butanol). Sol. CH_2Cl_2, $MeNO_2$, MeCN, MeOH. Mp 156°. Photosensitive - dec. by fluorescent light.

Martin, J.L. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 4493 (*synth*)
Burmeister, J.L. *et al*, *Inorg. Chim. Acta*, 1969, **3**, 105 (*synth, ir, uv-vis*)
Hiltunen, L. *et al*, *Acta Crystallogr., Sect. C*, 1987, **43**, 2063 (*cryst struct*)

IC-005613

$C_6N_6Pt^{2\ominus}$

Hexakis(cyano-*C*)platinate(2−), 9CI
Hexacyanoplatinate(IV)
[41517-45-7]

$[Pt(CN)_6]^{2\ominus}$ (O_h)

M 351.1 (ion)
Prepared form $CN^{\ominus}$ + $[PtI_6]^{2\ominus}$ or $[Pt(CN)_5I]^{2\ominus}$.
Di-K salt: [16920-94-8].
Colourless cryst. Sol. H_2O.

Swihart, D.L. *et al*, *Inorg. Chem.*, 1970, **9**, 1749 (*synth, uv-vis*)
Memering, M.N. *et al*, *Inorg. Chem.*, 1973, **12**, 2793 (*ir, raman*)
Weiss, J., *Z. Naturforsch., B*, 1974, **29**, 119 (*cryst struct*)
Pesek, J.J. *et al*, *J. Magn. Reson.*, 1977, **25**, 519 (*Pt-195 nmr*)
Pesek, J.J. *et al*, *Inorg. Chem.*, 1979, **18**, 924 (*cmr*)

IC-005614

$C_6N_6PtS_6^{2\ominus}$

Hexathiocyanatoplatinate(*IV*)(2−)
*Hexakis(thiocyanato-*S*)platinate*(IV)(*2*−)
[30068-96-3]

$[Pt(SCN)_6]^{2\ominus}$

M 543.5 (ion)
Ligand thought to coordinate through S. Light-sensitive anion. Props. not described.
Di-K salt: [17069-38-4].
Di-Na salt: [63128-72-3].
Norbury, A.H., *Adv. Inorg. Chem. Radiochem.*, 1975, **17**, 231.
Pesek, J.J. *et al*, *J. Magn. Reson.*, 1977, **25**, 519 (*Pt-195 nmr*)

IC-005615

$C_6N_6PtSe_6^{2\ominus}$

Hexaselenocyanatoplatinate(*IV*)(2−)
*Hexakis(selenocyanato-*Se*)platinate*(IV)(*2*−)

$[Pt(SeCN)_6]^{2\ominus}$

M 824.9 (ion)
Ligand probably coordinates through Se, but not confirmed by crystallography. Light-sensitive anion. Props. not described.
Di-K salt: [19610-63-0].
Bis-tetrabutylammonium salt: [18745-61-4].
Sabatini, A. *et al*, *Inorg. Chem.*, 1965, **4**, 959 (*ir*)
Swihart, D.L. *et al*, *Inorg. Chem.*, 1970, **9**, 1794 (*synth, uv-vis*)

IC-005616

$C_6N_6Re^{5\ominus}$

Hexakis(cyano-*C*)rhenate(*I*)(5−)
Hexacyanorhenate(*5*−)
[45047-06-1]

$[Re(CN)_6]^{5\ominus}$

M 342.3 (ion)
$Re(CN)_6^{6\ominus}$ has been reformulated to this sp.
K salt: [39700-07-7]. *Potassium hexacyanorhenate*(I).
Pentapotassium hexacyanorhenate
Synth. by reduction of $ReCl_6^{2\ominus}/CN^{\ominus}$ mixt. by $BH_4^{\ominus}$ or K/Hg. Yellow-green cryst. (H_2O). Ir $\nu_{C\equiv N}$ 1966 cm^{-1}. Isomorphous with Mn and Tc analogues.
[69290-36-4]

Schwochau, K. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **319**, 148 (*ir, raman*)
Krasser, W. *et al*, *Z. Naturforsch., A*, 1972, **27**, 1193 (*ir, raman*)
Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1411 (*synth, ir, props*)

IC-005617

$C_6N_6ReS_6^{3\ominus}$

Hexakis(thiocyanato-*N*)rhenate(*III*)(3−), 10CI
Hexaisothiocyanatorhenate(III)(*3*−)

$[Re(NCS)_6]^{3\ominus}$

M 534.7 (ion)
Octahedral.
Tris-tetrabutylammonium salt: [79244-72-7].
Synth. by reduction of $(Bu_4N)_2Re(NCS)_6$ with $N_2H_4.H_2O$, followed by addition of Bu_4NClO_4 in MeOH. Pale yellow cryst. Sol. MeCN.

Trop, H.S. *et al*, *Inorg. Chim. Acta*, 1981, **54**, L61 (*synth, ir, uv, props*)

IC-005618

$C_6N_6ReS_6^{2\ominus}$

Hexakis(thiocyanato-*N*)rhenate(*IV*)(2−), 10CI
Hexa(isothiocyanato)rhenate(IV)(*2*−)
[48072-47-5]

$[Re(NCS)_6]^{2\ominus}$

M 534.7 (ion)
Di-Cs salt:
$C_6Cs_2N_6ReS_6$ M 800.5
Synth. by fusion of K_2ReCl_6 with KSCN at 225°. Cs salt is obtd. by pptn. from H_2O. Dark brown solid. Sol. H_2O, EtOH, Et_2O, dil. acids and alkalis.
Di-Tl(I) salt: Synth. from $Cs_2Re(NCS)_6$ by pptn. with Tl acetate. Sl. sol. H_2O, EtOH.
Bis-tetrabutylammonium salt: [16985-65-2].
Synth. from $(Bu_4N)_2Re_2Cl_8$ and NaSCN in Me_2CO. Large red-brown cryst. Sol. H_2O.
Bis-Ph_4As salt: [16985-66-3].
Synth. from $(Bu_4N)_2Re_2Cl_8$, NaSCN, and Ph_4AsCl in MeOH.

Bailey, R.A. *et al*, *Inorg. Chem.*, 1967, **6**, 419, 2155 (*synth, props*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1967, **6**, 929 (*synth, props*)
Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 1160 (*synth, props*)

IC-005619

$C_6N_6Rh^{3\ominus}$

Hexakis(cyano-*C*)rhodate(3−)
[19356-46-8]

$[Rh(CN)_6]^{3\ominus}$

M 259.0 (ion)
Tri-K salt: [20792-40-9].
Prepd. by fusion of $RhCl_3$ with KCN. Red cryst. (H_2O).

Krauss, F. *et al*, *Z. Anorg. Allg. Chem.*, 1929, **179**, 357 (*synth*)
Jones, L.H., *J. Chem. Phys.*, 1964, **41**, 856 (*ir*)
Schmidtke, H.-H., *Z. Physik. Chem.*, 1964, **40**, 96 (*synth, uv*)
Pesek, J.J. *et al*, *Inorg. Chem.*, 1979, **18**, 924 (*cmr*)

IC-005620

$C_6N_6RhS_6^{3\ominus}$

Hexakis(thiocyanato-*S*)rhodate(*III*)(3−), 8CI
Hexathiocyanatorhodate(III)

$[Rh(SCN)_6]^{3\ominus}$ (O_h)

M 451.4 (ion)
Tri-K salt: Obt. when $RhCl_3$ dissolves in molten K[SCN] at 200°.
Tris-tetrabutylammonium salt: [17731-24-7].
Orange cryst. Sol. DMF.

Schmidtke, H.H. *et al*, *Helv. Chim. Acta*, 1967, **50**, 1631 (*synth, ir, props*)
Kerridge, D.H. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1579 (*synth*)

IC-005621

$C_6N_6RhSe_6^{3\ominus}$

Hexakis(selenocyanato-*N*)rhodate(*III*)(3−), 8CI
Hexaselenocyanatorhodate(III)(*3*−)

$[Rh(NCSe)_6]^{3\ominus}$

M 732.7 (ion)

Tris-tetrabutylammonium salt: [15617-40-0].
Dark red solid. Sol. $MeNO_2$.

Burmeister, J.L. *et al, Inorg. Chem.*, 1966, **5**, 1113 (*synth, uv, ir*)

IC-005622

$C_6N_6Ru^{3\ominus}$

Hexakis(cyano-*C*)ruthenate(*III*)(3−), 9CI
Hexacyanoruthenate(III)
[54692-27-2]

$[Ru(CN)_6]^{3\ominus}$ (O_h)

M 257.1 (ion)
Prepd. in aq. soln. by oxidising $[Ru(CN)_6]^{4\ominus}$ with H_2O_2, Ce(*IV*), Cl_2, O_3, PbO_2 or hydroxyl radicals.
Tris-Et₄N salt: [71514-21-1].
Yellow aq. soln.

DeFord, D.D. *et al, J. Am. Chem. Soc.*, 1951, **73**, 1469 (*synth, uv, electrochem*)
Kiss, A. *et al, Acta Chim. Acad. Sci. Hung.*, 1964, **40**, 397 (*uv*)
Waltz, W.L. *et al, Can. J. Chem.*, 1973, **51**, 2525 (*pulse radiolysis, uv*)
Vogler, A. *et al, Ber. Bunsenges. Phys. Chem.*, 1975, **79**, 301 (*synth*)
Moradpour, A. *et al, Nouv. J. Chim.*, 1978, **2**, 547 (*esr*)
Vogler, A. *et al, Inorg. Chim. Acta*, 1981, **53**, L215 (*uv, fluorescence*)
Crean, F.M. *et al, Inorg. Chem.*, 1984, **23**, 853 (*reactions*)

IC-005623

$C_6N_6RuS_6^{3\ominus}$

Hexakis(thiocyanato)ruthenate(*III*)(3−)
Hexathiocyanatoruthenate(III)(*3−*)
[52149-67-4]

$[Ru(NCS)_n(SCN)_{6-n}]^{3\ominus}$ ($1 \leqslant n \leqslant 6$)

M 449.5 (ion)
Prepd. as an isomeric mixture, which can be separated into four different components by high-voltage electrophoresis in water. All isomeric forms differ in their ir, Raman and uv spectra.
Tris-tetrabutylammonium salt (isomeric mixture): Prepd. by treating aq. $K_2[RuCl_6]$ with K[SCN], followed by addition of tetrabutylammonium bromide. Violet-blue solid. Insol. H_2O, sl. sol. Me_2CO, $MeNO_2$, CH_2Cl_2, DMF; sol. EtOH, $CHCl_3$. $\mu_{eff} = 2.02\mu_B$.

Mono-thiocyanato-N-form
*(Thiocyanato-*N*)pentakis(thiocyanato-*S*)ruthenate(3−), 9CI. Isothiocyanatopentathiocyanatoruthenate*(III)
Tris-tetrabutylammonium salt: [61202-48-0].
Blue-green cryst.

Bis-thiocyanato-N-form
*Bis(thiocyanato-*N*)tetrakis(thiocyanato-*S*)ruthenate(3−), 9CI. Diisothiocyanatotetrathiocyanatoruthenate*(III)
Stereoisomeric form not established.
Tris-tetrabutylammonium salt: [78510-95-9].
Blue-violet cryst.

Tris-thiocyanato-N-form
*Tris(thiocyanato-*N*)tris(thiocyanato-*S*)ruthenate(3−). Triisothiocyanatotrithiocyanatoruthenate*(III)
Tris-tetrabutylammonium salt: [78548-94-4].
Red-violet cryst.

Tetrakis-thiocyanato-N-form
*Tetrakis(thiocyanato-*N*)bis(thiocyanato-*S*)ruthenate(3−), 9CI. Tetraisothiocyanatodithiocyanatoruthenate*(III)
Tris-tetrabutylammonium salt: [63338-41-0].
Red-violet cryst.

Pentakis-thiocyanato-N-form
*Pentakis(thiocyanato-*N*)(thiocyanato-*S*)ruthenate(3−), 9CI. Pentaisothiocyanato(thiocyanato)ruthenate*(III)
Tris-tetrabutylammonium salt: [78548-98-8].
Prepd. by heating the corresp. salt of the isomeric mixt.

Hexakis-thiocyanato-N-form [48072-49-7]
*Hexakis(thiocyanato-*N*)ruthenate(3−), 9CI. Hexaisothiocyanatoruthenate*(III)
Tris-tetrabutylammonium salt: Prepd. by treating corresp. salt of $[Ru(NCS)_5(SCN)]^{3\ominus}$ with a 100-fold excess of tetrabutylammonium bromide in EtOH.
Tris[bis(triphenylphosphine)iminium] salt: Prepd. by heating the $[(Ph_3P)_2N]^{\oplus}$ salt of the isomeric mixt to >160°.
[61202-52-6, 61247-56-1, 78548-92-2, 78548-96-6]

Ogburn, S.C., *J. Am. Chem. Soc.*, 1926, **48**, 2493 (*soln chem*)
Forsythe, J.H.W. *et al, Talanta*, 1960, **3**, 324 (*soln chem*)
Schmidtke, H.-H., *J. Inorg. Nucl. Chem.*, 1966, **28**, 1735 (*synth*)
Schmidtke, H.-H., *Ber. Bunsenges. Phys. Chem.*, 1967, **71**, 1138 (*uv*)
Schmidtke, H.-H. *et al, Helv. Chim. Acta*, 1967, **50**, 1631 (*synth, uv, ir*)
Salzmann, J.J. *et al, Inorg. Chim. Acta*, 1969, **3**, 207 (*magnetism*)
Wajda, S. *et al, Nukleonika*, 1973, **18**, 407; *CA*, 1974, **80**, 125346 (*SCN$^{\ominus}$ exchange*)
Schwerdtfeger, H.-J. *et al, Angew. Chem., Int. Ed. Engl.*, 1977, **16**, 108 (*electrophoresis, ir*)
Fricke, H.H. *et al, Z. Naturforsch., B*, 1983, **38**, 917 (*synth, ir*)

IC-005624

$C_6N_6S_6Sc^{3\ominus}$

Hexakis(thiocyanato-*N*)scandate(3−)
Hexaisothiocyanatoscandate(III)
[45230-01-1]

$[Sc(NCS)_6]^{3\ominus}$

M 393.4 (ion)
Tri-Li salt: [27436-28-8].
Hygroscopic white cryst. + $10H_2O$. Sol. H_2O. Begins to dehydrate ~100°.
Tri-Na salt: [18538-77-7].
Hygroscopic white cryst. + $4H_2O$. Sol. H_2O. Begins to dehydrate at 40°.
Tri-K salt: [18538-78-8].
Hygroscopic white cryst. + $2H_2O$. Sol. H_2O. Dehydrates >190°, dec. > 280°.
Tri-Rb salt: [18538-79-9].
Hygroscopic white cryst. Sol. H_2O. Mp 180°. Dec. at 300°.
Tri-Cs salt: [18786-13-5].
Hygroscopic white cryst. Sol. H_2O. Mp 240°. Dec. >320°.
Tri-NH_4 salt: [27436-27-7].
White solid + $1H_2O$. Sol. H_2O. Mp 180°. Dehydrates >50°. Dec. >250°.
Tris-Me_4N salt: [29395-36-6].
White cryst. Mp 231° dec.
Tris-Et_4N salt: [29340-14-5].
White solid. Mp 221° dec.
Tris-phenanthrolinium(1+) salt: [29662-52-0].
White solid. Mp 189° dec.
Tris-Ph_4P salt: [65416-44-6].
White solid.

[27436-26-6]

Sarkar, P.B., *Ann. Chim.*, 1927, **8**, 207.
Urbain, G. *et al, Compt. Rend. Hebd. Seances Acad. Sci.*, 1927, **185**, 593.
Sas, T.M. *et al, Zh. Neorg. Khim.*, 1967, **12**, 2072; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 1090 (*synth, ir*)
Gulia, V.G. *et al, Zh. Neorg. Khim.*, 1970, **15**, 966; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 493 (*synth, dta*)

Eremin, Yu.G. *et al, Zh. Neorg. Khim.*, 1970, **15**, 2067; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1066 (*synth*)
Komissarova, L.N. *et al, Zh. Neorg. Khim.*, 1971, **16**, 2091, 2955, 3224; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 1115, 1570, 1708 (*synth, ir*)
Maltseva, V.S., *Zh. Neorg. Khim.*, 1977, **22**, 3160; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 1720 (*synth, ir*)
Hajeh, B. *et al, CA*, 1981, **95**, 107655 (*synth*)

IC-005625

$C_6N_6S_6Ta^{\ominus}$

Hexakis(thiocyanato-*N*)tantalate(*V*)(1−), 10CI
Hexakis(isothiocyanato)tantalate(V)(*1−*), *8CI. Hexaisothiocyanatotantalate*(V)(*1−*)
[16919-16-7]

$[Ta(NCS)_6]^{\ominus}$ (O_h)

M 529.4 (ion)
K salt: [16918-20-0].
$C_6KN_6S_6Ta$ M 568.5
Synth. from $TaCl_5$ + KNCS in MeCN. Orange solid. Sol. MeCN.
Tetrabutylammonium salt: [26032-40-6].
Synth. from K salt + tetrabutylammonium chloride in MeCN. Orange solid. Mp 130°.
Ph_4As salt: [19106-92-4].
Obt. by metathesis of K salt. Orange solid. Mp 226°.

Brown, T.M. *et al, J. Am. Chem. Soc.*, 1967, **89**, 5296 (*synth*)
Knox, G.F. *et al, Inorg. Chem.*, 1969, **8**, 1401 (*synth, uv-vis, ir*)
Sych, A.M. *et al, Koord. Khim.*, 1977, **3**, 226; *CA*, **86**, 132681h (*synth*)

IC-005626

$C_6N_6S_6Tc^{3\ominus}$

Hexakis(thiocyanato-*N*)technetate(*III*)(3−), 10CI
Hexaisothiocyanatotechnetate(III)
[72622-86-7]

$[Tc(NCS)_6]^{3\ominus}$ (O_h)

M 447.4 (ion)
Heptathiocyanatotechnetate(*III*) also claimed. Tc—N bond length equal to Fe—N in $[Fe(NCS)_6]^{3\ominus}$. λ_{max} ~400 nm.
Tris-tetrabutylammonium salt: [72622-87-8].
Yellow solid.
Tris-Ph_4As salt: [72622-88-9].
Yellow solid.

Trop, H.S. *et al, Inorg. Chem.*, 1980, **19**, 1105 (*synth, cryst struct, uv, ir, magnetism, conductivity, electrochem*)
Grases, F. *et al, Radiochim. Acta*, 1987, **42**, 47 (*ux, electrochem, props*)

IC-005627

$C_6N_6S_6Tc^{2\ominus}$

Hexakis(thiocyanato-*N*)technetate(*IV*)(2−), 10CI
Hexaisothiocyanatotechnetate(IV)(*2−*)
[45230-36-2]

$[Tc(NCS)_6]^{2\ominus}$ (O_h)

M 447.4 (ion)
Soln. chemistry of technetium thiocyanate complexes is complicated by ready redox and dissociation reactions. Synth. from hydrated TcO_2 + $(NH_4)NCS$ in dil. H_2SO_4, or by ligand exchange with $TcCl_6^{2\ominus}$ or $TcBr_6^{2\ominus}$. Purple anion. λ_{max} ~ 500 nm.
Bis-Me_4N salt: [40207-40-7].
Brown solid. Readily sol. Me_2CO, MeCN; spar. sol. dil. acids.
Bis-Ph_4As salt: Purple solid (forms 1:1 adduct with CH_2Cl_2). Paramagnetic, $\mu_{eff} = 4.10\mu_B$.

Bis-trioctylammonium salt: [17475-75-1].
Di-H compd.: [45230-38-4]. *Hexakis(thiocyanato-*N*) technetic*(IV) *acid*
$C_6H_2N_6S_6Tc$ M 449.4
[111256-71-4]

Schwochau, K. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 2249 (*synth, ux, ir, electrochem*)
Trop, H.S. *et al, J. Labelled Compd. Radiopharm.*, 1979, **16**, 82 (*synth, ux, electrochem*)
Trop, H.S. *et al, Inorg. Chem.*, 1980, **19**, 1105 (*synth, ux, electrochem*)
Williams, G.A. *et al, Aust. J. Chem.*, 1987, **40**, 27 (*synth, ir, cryst struct*)
Grases, F. *et al, Radiochim. Acta*, 1987, **42**, 47 (*ux, electrochem, props*)

IC-005628

$C_6N_6S_6Tc^{\ominus}$

Hexakis(thiocyanato-*N*)technetate(*V*)(1−)
Hexaisothiocyanatotechnetate(V)(*1−*)

$[Tc(NCS)_6]^{\ominus}$ (O_h)

M 447.4 (ion)
Reduction of $TcO_4^{\ominus}$ + $NCS^{\ominus}$ can give Tc^{V} or Tc^{IV}; $[Tc(NCS)_6]^{\ominus}$ can be pptd. as its $Tl^{\oplus}$ or $Me_4N^{\oplus}$ salt. A lipid-soluble Tc^{V} species is alleged to be $Tc(NCS)_5$. Synth. by $TcO_4^{\ominus}$ oxidation of $[Tc(NCS)_6]^{2\ominus}$. Used in spectrophotometric detn. of Tc; solvent extraction of Tc into alcohols, ethers, or ketones.
Me_4N salt: [22741-81-7].
Violet-black rhombohedral cryst. Spar. sol. H_2O; sol. Me_2CO, MeCN.

Hauck, J. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 927.
Schwochau, K. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 2249 (*synth, ux, ir, electrochem, conductance, magnetism, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, Suppl. Vol. 2, 1983, 200 (*rev*)
Cunningham, K.M. *et al, J. Nucl. Med.*, 1991, **73**, 878 (*synth, pharamco-kinetics*)

IC-005629

$C_6N_6S_6W$

Hexakis(thiocyanato-*N*)tungsten(*VI*)
Hexaisothiocyanatotungsten(VI). *Tungsten*(VI) *thiocyanate*

$W(NCS)_6$ (O_h)

M 532.3
Isol. as solvate from WCl_6 and NH_4SCN in dry Me_2CO, butanone or dioxan. Dark brown to dark green solid. $WO(NCS)_4$ also known.

Funk, H., *Z. Anorg. Allg. Chem.*, 1963, **324**, 168 (*synth*)

IC-005630

$C_6N_6S_6Zn^{4\ominus}$

Hexakis(thiocyanato-*N*)zincate(4−)
Hexa(isothiocyanato)zincate(4−)

$[Zn(NCS)_6]^{4\ominus}$

M 413.8 (ion)
Tetra-Na salt: [28237-76-5].
Cryst. + $2H_2O$.
Tetra-K salt: [26601-96-7].
Cryst. + $2H_2O$.
Tetra-Cs salt: [26601-97-8].
Cryst.
Tetra-acridinium salt: [53346-17-1].
Cryst.

[28630-78-6, 28630-79-7]

Kharitonov, Yu.Ya. *et al*, *Inorg. Nucl. Chem. Lett.*, 1970, **6**, 197; Kharitonov, Yu.Ya. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 614 (*synth, ir*)
Böhland, H. *et al*, *Z. Chem.*, 1974, **14**, 248 (*synth, ir*)

IC-005631

$C_6N_6Tc^{5\ominus}$

Hexakis(cyano-*C*)technetate(*I*)(5−)

Hexacyanotechnetate(I)(*5*−)

$[Tc(CN)_6]^{5\ominus}$ (O_h)

M 255.0 (ion)
Synth. from $TcO_4^{\ominus}$ by K/Hg redn. in presence of KCN (absence of air). Darkens on exp. to air; oxidises rapidly in aq. soln.
Penta-K salt: [41562-38-3].
Olive-green cryst. Spar. sol. H_2O.
Penta-Tl(I) *salt:* [93169-95-0].
Brick red solid. Insol. H_2O; sol. dil. acids.

Schwochau, K., *Ber. Kernforschungsanlage Juelich*, 1962, No. 68; *CA*, 1963, **58**, 8619e (*synth, struct, uv, ir*)
Schwochau, K. *et al*, *Z. Anorg. Allg. Chem.*, 1962, **319**, 148 (*synth, props*)

$C_6N_6Tc^{2\ominus}$ IC-005632

Hexakis(cyano-*C*)technetate(*IV*)(2−)

Hexacyanotechnetate(IV)(*2*−)

$[Tc(CN)_6]^{2\ominus}$ (O_h)

M 255.0 (ion)
Early report of prep. later questioned; see Heptakis(cyano-*C*)technetate(*III*)(4−), IC-005848. Synth. by reaction of $TcI_6^{2\ominus}$ with $CN^{\ominus}$.

Gmelin Handbook Inorg. Chem., Syst. No. 69; *Suppl. Vol.*, 1983, **2**, 200.

$C_6N_6Ti^{3\ominus}$ IC-005633

Hexakis(cyano-*C*)titanate(*III*)(3−), 10CI

Hexacyanotitanate(III)(*3*−)

$[Ti(CN)_6]^{3\ominus}$

M 203.9 (ion)
Tri-K salt: [14023-91-7].
$C_6K_3N_6Ti$ M 321.2
Synth. by heating $K_5Ti(CN)_8$ *in vacuo* at 280° and extracting with liq. NH_3. Black solid. Paramagnetic, $\mu_{eff} = 1.19\mu_B$.

Nicholls, D. *et al*, *Inorg. Chim. Acta*, 1980, **41**, 233 (*synth, ir, uv-vis, magnetism*)

$C_6N_6V^{4\ominus}$ IC-005634

Hexakis(cyano-*C*)vanadate(*II*)(4−), 11CI

Hexacyanovanadate(II)(*4*−)

[62073-22-7]

$[V(CN)_6]^{4\ominus}$ (O_h)

M 207.0 (ion)
Tetra-K salt: [17568-57-9]. *Potassium hexacyanovanadate*(II) ($K_4V(CN)_6$)
$C_6K_4N_6V$ M 363.4
Synth. by reducing $K_4[V(CN)_7]$ with K in liq. NH_3. Yellow-brown solid. Paramagnetic, $\mu_{eff} = 3.5\mu_B$, θ −52K.
Tetra-K salt, trihydrate: [27081-28-3].

Synth. by adding KCN to an aq. V(*II*) soln. formed by electrolytic reduction of $VOSO_4$. Orange-red solid. Dehydrates at 104°.

Griffiths, W.P. *et al*, *J. Chem. Soc. A*, 1970, 858 (*raman*)
Nast, R. *et al*, *Chem. Ber.*, 1971, **104**, 1709 (*synth, ir, magnetism*)
Dovgei, V.V. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 513 (*synth, ir, thermal dec*)
Jagner, S., *Acta Chem. Scand., Ser. A*, 1975, **29**, 255 (*cryst struct*)

$C_6N_7OV^{4\ominus}$ IC-005635

Hexakis(cyano-*C*)nitrosylvanadate(4−), 11CI

Hexacyanonitrosylvanadate(*4*−)

[67421-33-4]

$[V(NO)(CN)_6]^{4\ominus}$

M 237.0 (ion)
Pentagonal bipyramidal anion with axial NO.
Tri-K, Na salt: [66114-79-2].
Synth. by adding $NaClO_4$ to a soln. of $K_4[V(CN)_6NO]$ H_2O in H_2O. Yellow solid + $2H_2O$ (H_2O).
Tetra-K salt: [38883-01-1].
Synth. by passing H_2S into an aq. soln. of NH_4VO_3, KCN and NH_2OH. Yellow solid + $1H_2O$ (H_2O). The anhydrous salt is also known.
Tetra-K salt, hemi-KOH complex: [64397-57-5].
Cryst. + $\frac{1}{2}H_2O$.

[73889-65-3]

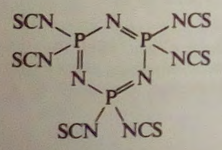
Mueller, A. *et al*, *Chem. Ber.*, 1972, **105**, 2419 (*synth*)
Drew, M.G.B. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 2838 (*synth, cryst struct, KOH compd*)
Jagner, S. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 653 (*synth, cryst struct*)

$C_6N_9P_3S_6$ IC-005636

2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexaisothiocyanato-1,3,5,2,4,6-triazatriphosphorine, 9CI, 8CI

Hexaisothiocyanatocyclotriphosphonitrile. Hexaisothiocyanatocyclotriphosphazene. 2,2,4,4,6,6-Hexaisothiocyanato-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,2,4,4,6,6-Hexaisothiocyanato-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine

[1858-42-0]

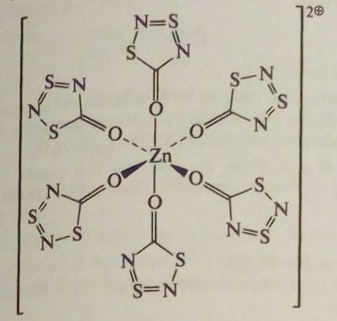


M 483.4
Triclinic; interatomic distances: P—N (ring) 158 , P—N (exocyclic) 163 pm. Synth. by reaction of $P_3N_3Cl_6$ + MSCN (M = Na, NH_4). Cryst. (heptane). Insol. H_2O, sol. Me_2CO, C_6H_6, v. sol. Et_2O. Mp 42°. Polym. at 150° → rubber.

Otto, R.J.A. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 5894 (*synth*)
Tesi, G. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 528 (*synth, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, C, 633 (*rev, bibl*)
Stahlberg, R. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2185 (*ir, raman*)
Fought, J.B. *et al*, *Inorg. Chem.*, 1970, **9**, 1656 (*cryst struct*)
Wagner, A.J. *et al*, *J. Chem. Soc. A*, 1971, 596 (*ms*)
Horn, H.G. *et al*, *Makromol. Chem.*, 1975, **176**, 1359 (*P-31 nmr, polymer*)
Walsh, E.J. *et al*, *Inorg. Chim. Acta*, 1976, **16**, L9 (*synth*)
Mason, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2337 (*N-14 nmr*)

$C_6N_{12}O_6S_{12}Zn^{2\oplus}$ IC-005637

Hexakis(5*H*-1,3,2,4-dithia(3-*S*^{IV})diazol-5-one-*O*)zinc(2+)



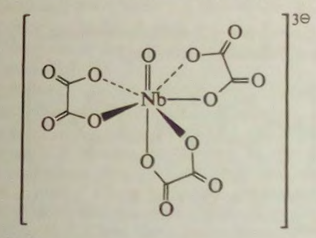
M 786.3 (ion)
Octahedral Zn.
Bis-hexafluoroarsenate: [83416-61-9].
Readily hydrol., colourless solid (SO_2). Insol. CH_2Cl_2. Mp 150°.

Roesky, H.W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 858 (*synth, ir, cryst struct*)

$C_6NbO_{13}^{3\ominus}$ IC-005638

Oxotris(oxalato)niobate(*V*)(3−)

Tris[*ethanedioato*(2−)-O,O′]*oxoniobate*(V)(*3*−), *11CI*



M 372.9 (ion)
Tri-NH_4 salt: [23388-19-4].
Synth. by dissolving Nb_2O_5 in an aq. mixt. of $H_2C_2O_4$ and $(NH_4)_2C_2O_4$. Colourless cryst. + $1H_2O$ (H_2O).
Tris-Ph_4P salt: [21393-49-7].
Synth. by dissolving Nb_2O_5 in aq. $H_2C_2O_4$ and adding Ph_4PCl. White solid (H_2O).
Ba salt (2:3): [82269-03-2].
Synth. by dissolving niobic acid in aq. $H_2C_2O_4$ and adding $Ba(NO_3)_2$. White solid + $8H_2O$. Dec. to $BaNb_2O_6$ at 550°.

Brničević, N. *et al*, *Inorg. Chem.*, 1968, **7**, 1936 (*synth, ir, Ph_4P salt*)
Mathern, G. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 1610 (*synth, cryst struct, NH_4 salt*)
Marta, L. *et al*, *Rev. Roum. Chim.*, 1982, **27**, 87; *CA*, **97**, 32645h (*synth, Ba salt*)

$C_6Nd_2O_{12}$ IC-005639

Neodymium(*III*) oxalate

Tris(*oxalato*)*dineodymium*(III). *Tris*(*ethanedioato*)*dineodymium*(III)

[1186-50-1]

$Nd_2(C_2O_4)_3$

M 552.5
Decahydrate: [14551-74-7].

$C_6H_{20}Nd_2O_{22}$ M 732.6
Isostructural series for Y, La - Ho. Violet cryst. 9-Coord., tricapped trigonal prism, Nd bound to $3H_2O$, 3 bidentate oxalate.

[10171-49-0, 28877-87-4]

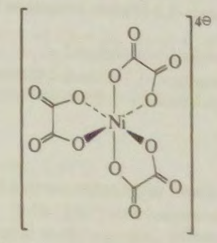
Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth, tga*)
Weigel, F. *et al*, *Z. Anorg. Allg. Chem.*, 1966, **345**, 119 (*synth, struct*)
Ollendorff, W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Hansson, E., *Acta Chem. Scand.*, 1970, **24**, 2969; 1973, **27**, 2852 (*cryst struct*)
Bezdenezhnykh, G.V. *et al*, *Zh. Neorg. Khim.*, 1971, **16**, 2943; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 1563 (*ir*)
Sharov, V.A. *et al*, *Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*tga, dta*)
Jeyaraj, G.L. *et al*, *Thermochim. Acta*, 1983, **71**, 345 (*dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6NiO_{12}^{4\ominus}$ IC-005640

Tris(oxalato)nickelate(*II*)(4−), 8CI

Tris(*ethanedioato*-O,O′)*nickelate*(II)(*4*−), *10CI*

[20710-68-3]



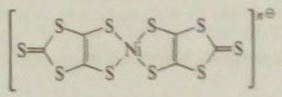
M 322.7 (ion)
Formed in soln. Not isol. Sol. H_2O.

Fridman, Ya.D. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 399 (*formn const*)
Hancock, R.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 67 (*uv*)

$C_6NiS_{10}^{\ominus}$ IC-005641

Bis[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-*S*^{4},*S*^{5}] nickelate(1−), 10CI

Bis(*dimercaptoisotrithione*)*nickelate*(*1*−)



n = 1

M 451.4 (ion)
Anions arranged in stacks. Synth. from Zn complex + $NiCl_2$ or $C_3S_5(Bu_4N)_2$ + $Ni^{2\oplus}$. Salts are organic electrical conductors.
Me_4N salt: [103171-60-4].
Large black or smaller green cryst.; black plates (MeCN). Monoclinic. Two forms α, β. Superconductor when under pressure.
Et_4N salt: [103171-57-9].
Large black cryst. Disordered semiconductor.
Pr_4N salt: [118395-35-0].
Large black cryst. or smaller green cryst. Struct. non-planar around Ni.
Tetrabutylammonium salt: [68401-88-7].

Greenish-black cryst. (Me_2CO/MeOH); black plates or needles. V. sol. Me_2CO; sol. MeOH; insol. H_2O. Mp 190-193°. μ_{eff} = 1.90μ_B.

[105029-70-7, 120141-29-9, 120141-30-2, 120156-10-7]

Steinecke, G. *et al*, *Phosphorus Sulfur*, 1979, **7**, 49 (*synth, uv-vis*)
Kirmse, R. *et al*, *Inorg. Chem.*, 1980, **19**, 2679 (*synth, magnetism*)
Papassiliou, G.C. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1200 (*synth, props*)
Poleschner, H. *et al*, *J. Prakt. Chem.*, 1983, **325**, 957 (*synth, ir*)
Sakamoto, Y. *et al*, *Inorg. Chim. Acta*, 1986, **113**, 137 (*ir, pe, esr*)
Groeneveld, L.R. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1986, **105**, 507 (*synth, cryst struct*)
Mentsafos, D. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 1550 (*cryst struct*)
Van Diemen, J.H. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 1898 (*synth, cryst struct*)
Kramer, G.J. *et al*, *J. Phys. Chem.*, 1988, **21**, 6085 (*electrical props*)
Kajita, K. *et al*, *Solid State Commun.*, 1988, **65**, 361 (*electrical props*)
Kobayashi, K. *et al*, *Synth. Met.*, 1988, **27**, B339 (*cryst struct, electrical props*)
Kato, R. *et al*, *Synth. Met.*, 1988, **27**, B359 (*salts, synth, cryst structs*)

$C_6NiS_{10}^{2\ominus}$ IC-005642

Bis[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-S^4,S^5] nickelate(2−)

Bis(isotrithionedithiolato)nickelate(2−)

As Bis[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-S^4,S^5] nickelate(1−), IC-005641 with

$n = 2$

M 451.4 (ion)

Nearly square planar coordination around Ni.

Bis(tetrabutylammonium) salt: [72022-67-4].
Dark green needles (isopropanol) or larger black cryst. Sol. Me_2CO. Mp 197-199°. Diamagnetic; shows unexpectedly high electrical conductivity.

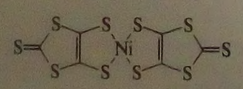
[105005-65-0, 105057-97-4, 105177-35-3, 107766-73-4]

Lundqvist, O. *et al*, *Acta Chem. Scand., Ser. A*, 1979, **33**, 445; 1982, **36**, 855 (*synth, cryst struct*)
Steinecke, G. *et al*, *Phosphorus Sulfur*, 1979, **7**, 49 (*synth, cryst struct, uv-vis*)
Zhu, D. *et al*, *Kexue Tongbao (Chin. Ed.)*, 1986, **31**, 382 (*ir, pe*)
Papavassilou, G.C. *et al*, *Chem. Scr.*, 1987, **27**, 261 (*synth*)
Kobayashi, A. *et al*, *Solid State Commun.*, 1987, **62**, 57 (*electronic struct*)

C_6NiS_{10} IC-005643

Bis[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-S^4,S^5] nickel

[72018-82-7]



M 451.4

Centrosymmetric; almost planar struct. around Ni. Partially oxidised spp. investigated as materials for molecular electronics. Platelets.

Valade, L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 783 (*synth, cryst struct*)
Kosayashi, A. *et al*, *Solid State Commun.*, 1987, **62**, 57 (*electronic struct*)
Underhill, A.E., *Chem. Br.*, 1991, **27**, 708 (*rev*)

$C_6Ni_2O_6^{2\ominus}$ IC-005644

Hexacarbonyldinickelate(2−), 9CI

[80790-08-5]

$[Ni_2(CO)_6]^{2\ominus}$

M 285.4 (ion)

Di-Na salt: Obt. only in NH_3 soln. on reduction of $Ni(CO)_4$ by Na. Readily condenses furtherby CO loss, or undergoes ammoniolysis to $Ni_2(CO)_6H_2$.

Behrens, H. *et al*, *Chem. Ber.*, 1961, **94**, 1391 (*synth*)
Pacchoni, G. *et al*, *J. Organomet. Chem.*, 1982, **224**, 89.

C_6O IC-005645

Carbon oxide (C_6O)

6-Oxo-1,2,3,4,5-hexapentaenylidene, 12CI. Hexacarbon monoxide

[112022-62-5]

$:C{=}C{=}C{=}C{=}C{=}C{=}O$

M 88.0

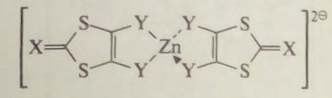
Triplet. Formed by vaporising graphite in CO/Ne. Known only in a Ne or Ar matrix.

Van Zee, R.J. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 609 (*matrix, isol, esr*)

$C_6O_2S_8Zn^{2\ominus}$ IC-005646

Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-S^4,S^5] zincate(2−)

Bis(1,3-dithiole-2-one-4,5-dithiolato)zincate(2−). Bis(2-oxo-1,3-dithiole-4,5-dithiolato)zincate(2−)



X = O, Y = S

M 425.9 (ion)

Bis-Me_4N salt: Cryst. Mp 225° dec.

Bis-tetrabutylammonium salt: [97689-29-7]. Red cryst. Mp 136° dec.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1988, **567**, 131 (*synth, ir, cmr*)
Ikegawa, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 262 (*synth*)

C_6O_5SW IC-005647

(Carbonothioyl)pentacarbonyltungsten, 9CI

Thiocarbonylpentacarbonyltungsten

[50358-92-4]

$(OC)_5WCS$

M 367.9

Yellow cryst. (hexane).

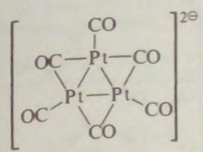
Angelici, R.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 7516 (*props*)
Angelici, R.J. *et al*, *Inorg. Chem.*, 1976, **15**, 1089 (*synth*)
Fenske, R.F. *et al*, *Inorg. Chem.*, 1976, **15**, 2015 (*struct*)
Angelici, R.J. *et al*, *Inorg. Chem.*, 1976, **15**, 2403 (*props*)
Poliakoff, M., *Inorg. Chem.*, 1976, **15**, 2892 (*ir*)
Butler, I.S., *Acc. Chem. Res.*, 1977, **10**, 359 (*synth, props*)

$C_6O_6Pt_3^{2\ominus}$ IC-005648

Tri-μ-carbonyltricarbonyltriplatinate(2−)

Hexacarbonyltriplatinate(2−)

[63993-21-5]



M 753.3 (ion)

Di-K salt: Pink-red soln., dec. on attempt to precipitate.

Longoni, G. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 7225 (*synth, ir*)
Brown, C. *et al*, *J. Organomet. Chem.*, 1979, **181**, 233 (*nmr*)

$C_6O_6Re^{\ominus}$ IC-005649

Hexacarbonylrhenium(*I*)(1+)

Rhenium hexacarbonyl(1+)

[21266-11-5]

$[Re(CO)_6]^{\oplus}$ (O_h)

M 354.2 (ion)

Hexafluorophosphate: [38656-75-6].
White air-stable cryst.

Perchlorate: Synth. from $Re(CO)_5Cl$, ACl_3, CO and $HClO_4$. White cryst. (EtOH).

Pentafluorooxorhenate(VI)(1−): [62259-54-5].
$C_6F_5O_7Re_2$ M 651.4
Synth. by part. hydrol. of $Re(CO)_5F.ReF_5$. Pale green cryst. solid. Sol. HF. Ir $\nu_{Re=O}$ 997 cm^{-1}, ν_{CO} 2193sh, 2125sh, 2084vs, 2063sh, 2044sh cm^{-1} (nujol).

μ-Fluorodecafluorodirhenate(V)(1−): see *μ-Fluorodecafluorodirhenate(V)(1−), IC-018817*

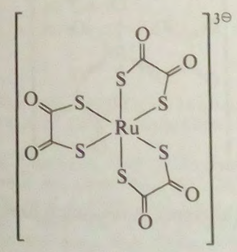
Hieber, W. *et al*, *Z. Naturforsch., B*, 1961, **16**, 709 (*synth*)
Kruck, T. *et al*, *Chem. Ber.*, 1963, **96**, 3028; 1966, **99**, 1153 (*synth*)
Nyholm, R.S. *et al*, *J. Chem. Soc.*, 1965, 6564 (*synth, perchlorate*)
Abel, E.W. *et al*, *J. Mol. Spectrosc.*, 1969, **30**, 29 (*ir*)
Bruce, D.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2230; 1978, 1627 (*deriv, synth, ir, raman, props, cryst struct*)

$C_6O_6RuS_6^{3\ominus}$ IC-005650

Tris(dithiooxalato)ruthenate(*III*)(3−)

Tris[ethanebis(thioato)(2−)-S,S′]ruthenate(3−), 9CI

[43190-69-8]



M 461.5 (ion)

Tris-Ph_4As salt: Prepd. by treating aq. $RuCl_3$ with $K_2[S_2C_2O_2]$, followed by $[AsPh_4]Cl$.

DeSimone, R.E., *J. Am. Chem. Soc.*, 1973, **95**, 6238 (*synth, esr*)

$C_6O_6Ti^{2\ominus}$ IC-005651

Hexacarbonyltitanate(2−)

$[Ti(CO)_6]^{2\ominus}$

M 215.9 (ion)

Di-K salt, bis(15-crown-5) complex: Deep-red cryst. (MeCN/DME). Dec. at 180-182°.

Di-K salt, bis([2.2.2]cryptand) complex: Dark-violet cryst. (MeCN/THF). Mp 216-217° dec.

Chi, K.M. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 303 (*synth, ir, cmr, Ti nmr*)

$C_6O_6V^{\ominus}$ IC-005652

Hexacarbonylvanadate(1−)

$[V(CO)_6]^{\ominus}$

M 219.0 (ion)

Na salt, bis(diglyme) complex: [15531-13-2].
Yellow solid. Sol. H_2O. Mp 173-176° dec. (under N_2).

Tris(triphenylphosphine)copper(I) salt: [98542-02-0].
$C_{60}H_{45}CuO_6P_3V$ M 1069.4
Bright yellow cryst. (toluene). Ir ν_{CO} ~1850 cm^{-1}. Struct. consists of discrete trigonal cations and octahedral anions.

Werner, R.P.M. *et al*, *Chem. Ind. (London)*, 1961, 144 (*synth, ir*)
Doyle, G. *et al*, *Organometallics*, 1985, **4**, 2201 (*synth, ir, cryst struct, Cu-contg deriv*)
Kowaleski, R.M. *et al*, *Organometallics*, 1988, **7**, 1425 (*esr*)

C_6O_6W IC-005653

Tungsten carbonyl, 9CI

Hexacarbonyltungsten. Tungsten hexacarbonyl

[14040-11-0]

$W(CO)_6$ (O_h)

M 351.9

Important starting material. Air-stable, colourless, odourless cryst. Sl. sol. hexane. Mp 150° dec.

[17594-12-6, 25941-11-1, 25941-12-2]

Arnesen, S.P. *et al*, *Acta Chem. Scand.*, 1966, **20**, 2711 (*ed*)
Jones, L.H. *et al*, *Inorg. Chem.*, 1969, **11**, 2349 (*ir*)
Beneze, L., *J. Organomet. Chem.*, 1972, **37**, C37 (*struct*)
Braterman, P.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1027 (*nmr*)
Dellien, I. *et al*, *Chem. Rev.*, 1976, **76**, 283.
Hagen, A.P. *et al*, *Inorg. Chem.*, 1978, **17**, 1369 (*synth, bibl*)
Keiter, R.L. *et al*, *J. Organomet. Chem.*, 1984, **258**, C34 (*W-183 nmr*)

$C_6O_6Zr^{2\ominus}$ IC-005654

Hexacarbonylzirconate(2−)

$[Zr(CO)_6]^{2\ominus}$

M 259.2 (ion)

First binary carbonylzirconium complex; stabilized by use of crown-ether with counter-cation.

Di-K salt, bis(15-crown-5) complex: [111004-77-4]. Extremely air-sensitive dark-purple microcryst. (MeCN/THF). Dec. at 140°. Ir ν_{CO} 1757 cm^{-1}.

Chi, K.M. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1987, **26**, 1190 (*synth, ir, cmr, Zr-91 nmr*)

IC-005655

$C_6O_{12}Pm_2$

Promethium(*III*) oxalate

Tris(oxalato)dipromethium(III). *Tris(ethanedioato) dipromethium*(III)

$Pm_2(C_2O_4)_3$

M 553.8

Decahydrate: [14462-37-4].
$C_6H_{20}O_{22}Pm_2$ M 734.0
Rose-violet cryst. Prob. 9-coordinate by analogy with various analogues. Evidence exists for trihydrate in tga.

[25880-55-1]

Parker, G.W., *J. Am. Chem. Soc.*, 1950, **72**, 2834 (*synth*)
Weigel, F. *et al*, *Z. Anorg. Allg. Chem.*, 1966, **345**, 119 (*synth, struct*)
McNeilly, C.F. *et al*, *Therm. Anal., Proc. Int. Conf., 2nd, 1968*,
Worcester Mass, 1968, **2**, 727; *CA*, 1970, **72**, 6767 (*tga*)

IC-005656

$C_6O_{12}Pr_2$

Prasedymium(*III*) oxalate

Tris(oxalato)dipraseodymium(III). *Tris(ethanedioato) dipraseodymium*(III)

[57417-70-6]

$Pr_2(C_2O_4)_3$

M 545.8

Decahydrate: [24992-60-7].
$C_6H_{20}O_{22}Pr_2$ M 726.0
Green cryst. 9-Coordination presumed, by analogy with Nd analogue. $\mu_{eff} = 3.45\mu_B$ (293K).

[57417-70-6, 70063-10-4]

Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth, tga*)
Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Möbius, R. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1601 (*dta*)
Ollendorff, W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*tga, dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

IC-005657

$C_6O_{12}Pu_2$

Plutonium(*III*) oxalate

$Pu_2(C_2O_4)_3$

M 742.1

Anhyd. compd. possibly obtd. from hydrate in air >225°. At 270°, oxidised to PuO_2. Insolubility utilized in Pu purification.

Decahydrate: Blue-green solid. Insol. H_2O.
Undecahydrate: Brilliant dark green to pale green cryst. Insol. H_2O. Loses H_2O on heating at 220°. Dec. at 300°.

[50647-42-2]

Chackraburtty, D.M., *Acta Crystallogr.*, 1963, **16**, 834
Jenkins, I.L. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **27**, 77, 81.
Burney, G.A. *et al*, *Inorg. Nucl. Chem. Lett.*, 1967, **3**, 79 (*soly*)
Gmelin Handbook Inorg. Chem., Syst. No. 71, 1972, **C**, 236 (*rev*)
Cleveland, J.M., *The Chemistry of Plutonium*, American Nuclear Society, 1979, 398.

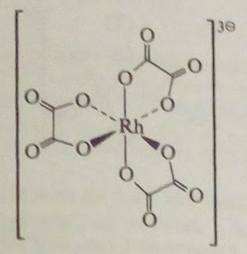
$C_6O_{12}Rh^{3\ominus}$

IC-005658

Tris(oxalato)rhodate(*III*)(3−), 8CI

Tris[1,2-ethanedioato(2−)-O,O′]rhodate(3−), 10CI, 9CI

[18307-26-1]



M 366.9 (ion)
Distorted octahedral struct. Can be resolved as strychnine salt.

A-form

Tri-K salt: [26934-21-4].
Red cryst. + $1H_2O$. $[\alpha]_D$ + 0°, $[\alpha]_D$ + C −26.4°, $[\alpha]_D$ + E +114.4°.

A-form

Tri-K salt: [58958-00-2].
Red prismatic cryst. + $1H_2O$. $[\alpha]_D$ + C +30°, $[\alpha]_D$ + E −124°.

[15602-35-4, 19710-48-6, 37433-41-3, 88055-93-0]

Werner, A., *Ber.*, 1914, **47**, 1955 (*synth, resoln*)
Dwyer, F.P. *et al*, *J. Phys. Chem.*, 1956, **60**, 1331 (*uv, ord*)
Wendlandt, W.W. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **21**, 69 (*synth, thermal anal*)
Gillard, R.D. *et al*, *J. Chem. Soc. A*, 1969, 3006 (*cryst struct*)
Dalzell, B.C. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 4298 (*cryst struct*)
Mathieu, J.P., *J. Raman Spectrosc.*, 1973, **1**, 47 (*raman, ir*)
Gouternon, J., *J. Inorg. Nucl. Chem.*, 1976, **38**, 55 (*ir, resoln*)
Okazaki, H., *J. Sci. Hiroshima Univ. Ser. A: Phys. Chem.*, 1983, **47**, 1 (*cryst struct, abs config, K salt*)

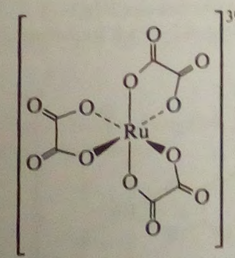
$C_6O_{12}Ru^{3\ominus}$

IC-005659

Tris(oxalato)ruthenate(*III*)(3−)

Tris[ethanedioato(2−)-O,O′]ruthenate(III)(3−)

[25072-75-7]



M 365.1 (ion)
Octahedral. All attempts at resolution have been unsuccessful.

Tri-K salt, trihydrate:
$C_6H_6K_3O_{15}Ru$ M 536.4
Synthetic reagent. Green salt (EtOH aq.).
Tri-K salt, 4.5 hydrate: Green salt (H_2O). $\mu_{eff} = 2.04\mu_B$.
Tri-NH_4 salt: Yellow salt + 1.5 H_2O (H_2O). $\mu_{eff} = 2.02\mu_B$.

Charonnat, R., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1924, **178**, 1279 (*synth*)
Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 124, 156, 225 (*synth*)
Dwyer, F.P. *et al*, *J. Phys. Chem.*, 1956, **60**, 1331 (*synth*)

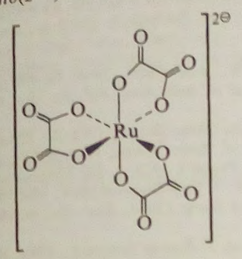
Wagnerová, D.M., *Collect. Czech. Chem. Commun.*, 1962, **27**, 1130 (*electrochem*)
Olliff, R.W. *et al*, *J. Chem. Soc.*, 1964, 2417, 2467 (*magnetism, uv*)
Bittel, R. *et al*, *Bull. Soc. Chim. Fr.*, 1969, 3830 (*synth*)
Key, D.L. *et al*, *J. Chem. Soc. A*, 1971, 371 (*synth, magnetism*)
DeSimone, R.E., *J. Am. Chem. Soc.*, 1973, **95**, 6238 (*esr*)
Poon, C.-K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1336 (*reactions*)
Olubuyide, O. *et al*, *Inorg. Chem.*, 1986, **25**, 4798 (*reaction*)
Kaziro, R. *et al*, *Inorg. Chim. Acta*, 1989, **164**, 85 (*synth, reduction*)

IC-005660

$C_6O_{12}Ru^{2\ominus}$

Tris(oxalato)ruthenate(*IV*)(2−)

Tris[ethanedioato(2−)-O,O′]ruthenate(IV)(2−)



M 365.1 (ion)
Octahedral anion. Electrochemically reduced to Tris(oxalato)ruthenate(*III*)(3−), IC-005659.

Di-K salt: Prepd. by the oxidation of $K_3[Ru(C_2O_4)_3]$ with H_2O_2. Black solid.

Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 168 (*synth*)
Wagnerová, D.M., *Collect. Czech. Chem. Commun.*, 1962, **27**, 1130 (*electrochem*)

IC-005661

$C_6O_{12}Sc_2$

Scandium(*III*) oxalate

Tris(oxalato)discandium(III). *Tris(ethanedioato) discandium*(III)

[13419-51-7]

$Sc_2(C_2O_4)_3$

M 353.9

Hexahydrate: [35138-42-2].
$C_6H_{12}O_{18}Sc_2$ M 462.0
Colourless cryst.
Decahydrate: [30618-34-9].
$C_6H_{20}O_{22}Sc_2$ M 534.1
Efflorescent, colourless cryst. 8-Coord. dodecahedral struct.

[51407-18-2]

Nilson, L.F., *Chem. Ber.*, 1880, **13**, 1439 (*synth*)
Štěrbo-Böhm, J.S. *et al*, *Collect. Czech. Chem. Commun.*, 1929, **1**, 1 (*synth*)
Dupuis, J., *Anal. Chim. Acta*, 1949, **3**, 183 (*synth*)
Klein, M.P. *et al*, *J. Am. Chem. Soc.*, 1951, **73**, 1364 (*synth*)
Wendlandt, W.W. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **17**, 273.
Head, E.L. *et al*, *J. Inorg. Nucl. Chem.*, 1964, **26**, 515 (*dta*)
Watanabe, M. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 3604 (*synth*)
Hansson, E., *Acta Chem. Scand.*, 1972, **26**, 1337 (*cryst struct*)
Koblova, O.E. *et al*, *Zh. Neorg. Khim.*, 1977, **22**, 1230; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 670 (*ir*)
Thomas, Y. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1978, **286**, 119 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 113 (*rev, bibl*)

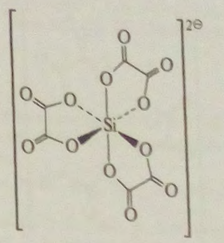
$C_6O_{12}Si^{2\ominus}$

IC-005662

Tris(oxalato)silicate(2−)

Tris[ethanedioato(2−)-O,O′]silicate(2−)

[29997-08-8]



M 292.1 (ion)
Prepd. from $SiCl_4$ + $Ag_2C_2O_4$.

Bis-Me_4N salt: [38587-08-5].
Mp 276-277° dec.
Bis-Et_4N salt: [22685-90-1].
White needles (EtOH). Mp 169-170°, Mp 235°.
Bis-Et_3NH salt: [38683-96-4].
Mp 115-117°.
Bis-tetrabutylammonium salt: [38587-10-9].
Mp 113°.
Bis-$EtPh_3P$ salt: [38587-11-0].
Mp 140-141°.

Dean, P.A.W. *et al*, *J. Chem. Soc. A*, 1969, 363 (*synth, ir, raman*)
Schott, G. *et al*, *Z. Anorg. Allg. Chem.*, 1972, **391**, 27 (*synth, ir*)
Cella, J.A. *et al*, *J. Organomet. Chem.*, 1980, **186**, 13 (*Si-29 nmr*)

IC-005663

$C_6O_{12}Sm_2$

Samarium(*III*) oxalate

Tris(oxalato)disamarium(III). *Tris(ethanedioato) disamarium*(III)

[3252-68-4]

$Sm_2(C_2O_4)_3$

M 564.7

Decahydrate: [14175-03-2].
$C_6H_{20}O_{22}Sm_2$ M 744.9
Bright yellow cryst.

[10171-50-3]

Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58; 1959, **31**, 408 (*synth, dta, tga*)
Grzymalski, Z. *et al*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Weigel, F. *et al*, *Z. Anorg. Allg. Chem.*, 1966, **345**, 119 (*struct*)
Weigel, F. *et al*, *Acta Crystallogr.*, 1967, **22**, 923 (*struct*)
Ollendorff, W. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Thomas, Y. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. B*, 1978, **286**, 119 (*ir, raman*)
Sharov, V.A. *et al*, *Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Thomas, Y. *et al*, *Physica C: (Amsterdam)*, 1979, **98**, 131 (*ir, raman*)
Fuller, M.J. *et al*, *J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al*, *J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

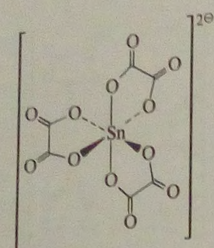
IC-005664

$C_6O_{12}Sn^{2\ominus}$

Tris(oxalato)stannate(*IV*)(2−)

Tris[ethanedioato(2−)-O,O′]stannate(2−), 1ICI

[31974-78-4]



M 382.7 (ion)

Bis-Et_4N salt: [22685-91-2].
White cryst. Mp 202°.

[88031-31-6]

Dean, P.A. *et al, J. Chem. Soc. A*, 1969, 363 (*synth, ir, raman*)
Antanov, P.G. *et al, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol.*, 1988, **31**, 23 (*synth, ir, uv, mössbauer*)

IC-005665

$C_6O_{12}Tb_2$

Terbium(*III*) oxalate

Tris(oxalato)diterbium(III). *Tris(ethanedioato)diterbium*(III)

[996-33-8]

$Tb_2(C_2O_4)_3$

M 581.9

Decahydrate: [24670-06-2].
$C_6H_{20}O_{22}Tb_2$ M 762.0
Presumed 9-coord. from struct. of Nd analogue. μ_{eff} = 9.63μ_B.

[58176-68-4]

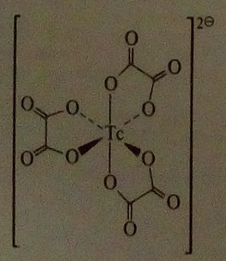
Wendlandt, W.W., *Anal. Chem.*, 1959, **31**, 408 (*dta, synth*)
Grzymalski, Z. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Ollendorff, W. *et al, Inorg. Nucl. Chem. Lett.*, 1969, **5**, 263 (*struct*)
Hansson, E. *et al, Acta Chem. Scand.*, 1973, **27**, 823 (*synth*)
Sharov, V.A. *et al, Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Fuller, M.J. *et al, J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al, J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

IC-005666

$C_6O_{12}Tc^{2\ominus}$

Tris(oxalato)technetate(*IV*)(2−)

Tris[ethanedioato(2−)-O,O′]technetate(2−)



M 362.9 (ion)
Octahedral anion. Synth. from $[TcBr_6]^{2\ominus}$ and oxalic acid.
Bis-Ph_4As salt: [111919-70-1].

Yellow solid. Mp *ca.* 260° dec.

Colmanet, S.F. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 2305 (*synth, ir, cryst struct*)

$C_6O_{12}Tm_2$

Thulium(*III*) oxalate IC-005667

Tris(oxalato)dithulium(III). *Tris(ethanedioato)dithulium*(III)

$Tm_2(C_2O_4)_3$

M 601.9

Hexahydrate: [26677-68-9].
$C_6H_{12}O_{18}Tm_2$ M 710.0
Green solid. Presumed 8-coord. by comparison with Yb analogue. μ_{eff} = 7.47μ_B.

[13285-38-6]

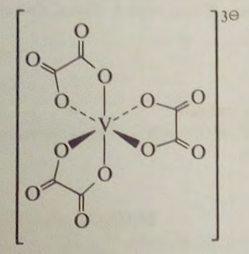
Wendlandt, W.W., *Anal. Chem.*, 1959, **31**, 408 (*synth, tga*)
Grzymalski, Z. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Hansson, E., *Acta Chem. Scand.*, 1973, **27**, 823 (*struct*)
Sharov, V.A. *et al, Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Fuller, M.J. *et al, J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al, J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6O_{12}V^{3\ominus}$ IC-005668

Tris(oxalato)vanadate(*III*)(3−), 8CI

Tris[ethanedioato(2−)-O,O′]vanadate(III)(3−), *11CI*

[20480-84-6]



Λ-form

M 315.0 (ion)
Octahedral. The Λ-form has been obt. and its spectra studied.

Tri-K salt: [36490-68-3].
Synth. by heating the trihydrate. Green solid.
Tri-K salt, trihydrate: [14023-93-9].
Synth. e.g. from $VCl_3.6H_2O$ or and $K_2C_2O_4$ in H_2O. Dark green solid (H_2O). Paramagnetic, μ_{eff} = 2.80μ_B (304K), 2.75μ_B (85K).
Tris-hydrazinium(1+) salt: [70515-93-4].
Synth. from $VCl_3.6H_2O$ and hot aq. $(N_2H_5)_2C_2O_4$. Green solid + $1N_2H_4$.

[57128-49-1]

Machin, D.J. *et al, J. Chem. Soc. A*, 1967, 1498 (*synth, magnetism*)
Gillard, R.D. *et al, J. Chem. Soc. A*, 1969, 3006 (*ir, raman, uv-vis, struct*)
Nagase, K., *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2166 (*thermal anal*)
Ahmed, N. *et al, Inorg. Chim. Acta*, 1975, **14**, 215 (*ord, cd*)
Gillard, R.D. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 594 (*resoln*)
Povarova, N.V. *et al, Koord. Khim.*, 1979, **5**, 381; *CA*, **91**, 129188x (*synth, magnetism*)

IC-005669

$C_6O_{12}Y_2$

Yttrium(*III*) oxalate

Tris(oxalato)diyttrium(III). *Tris(ethanedioato)diyttrium*(III)

[867-68-5]

$Y_2(C_2O_4)_3$

M 441.8

Hexahydrate:
$C_6H_{12}O_{18}Y_2$ M 549.9
Colourless solid. Presumed 8-coord. by analogy with Yb analogue. Other hydrates also known.

[13266-82-5, 18972-09-3, 58176-71-9]

Wendlandt, W.W., *Anal. Chem.*, 1958, **30**, 58 (*synth, tga*)
Watanabe, M. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 3604 (*struct*)
Fuller, M.J. *et al, J. Less-Common Met.*, 1980, **70**, 127 (*tga, dta*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)

IC-005670

$C_6O_{12}Yb_2$

Ytterbium(*III*) oxalate

Tris(oxalato)diytterbium(III). *Tris(ethanedioato) diytterbium*(III)

[996-34-9]

$Yb_2(C_2O_4)_3$

M 610.1

Hexahydrate: [30618-32-7].
$C_6H_{12}O_{18}Yb_2$ M 718.2
Part of an isomorphous series Er → Lu (isotypic with Sc). Colourless solid. 8-Coord. ($2H_2O$, 3 bidentate oxalates).

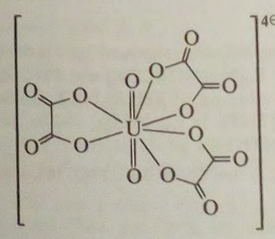
[13285-37-5, 58176-74-2]

Wendlandt, W.W., *Anal. Chem.*, 1959, **31**, 408 (*synth, tga*)
Grzymalski, Z. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 475 (*ir*)
Watanabe, M. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 3604.
Hansson, E., *Acta Chem. Scand.*, 1973, **27**, 823 (*cryst struct, synth*)
Sharov, V.A. *et al, Koord. Khim.*, 1979, **5**, 653; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1979, **5**, 512 (*magnetism*)
Fuller, M.J. *et al, J. Less-Common Met.*, 1980, **70**, 127 (*dta, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1984, **D5**, 124 (*rev, bibl*)
Morris, D.E. *et al, J. Raman Spectrosc.*, 1988, **19**, 231 (*ir, raman*)

$C_6O_{14}U^{4\ominus}$ IC-005671

Tris(oxalato)dioxouranate(*VI*)(4−)

Tris[ethanedioato(2−)-O,O′]dioxouranate(4−). Trioxalatouranyl(1−)



M 534.0 (ion)
Hexagonal bipyramidal anion.
Tetra-NH_4 salt: [17476-37-8].
Pale yellow cryst.

Alcock, N.W., *J. Chem. Soc., Dalton Trans.*, 1973, 1610 (*synth, cryst struct, uv-vis*)

$C_6S_6Se_4Zn^{2\ominus}$

IC-005672

Bis(1,3-dithiole-2-thione-4,5-diselenolato)zincate(2−)

Bis[4,5-diselenyl-1,3-dithiole-2-thionato(2−)-Se,^{4},Se^5] zincate(2−)

As Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-S^4,S^5] zincate(2−), IC-005646 with

X = S, Y = Se

M 645.6 (ion)

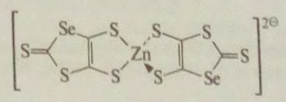
Bis-tetrabutylammonium salt: [119509-05-6].
Dark red cryst. (Me_2CO/2-propanol). Sol. $CHCl_3$. Mp 160-163° dec.

Olk, R.-M. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1984, **14**, 915 (*synth*)
Olk, R.-M. *et al, Z. Chem.*, 1988, **28**, 304 (*synth*)
Olk, R.-M. *et al, Z. Anorg. Allg. Chem.*, 1989, **577**, 206 (*synth, ir, uv-vis, cmr*)

$C_6S_9Se_2Zn^{2\ominus}$ IC-005673

Bis(1,3-thiaselenole-2-thione-4,5-dithiolato)zincate(2−)

Bis[4,5-dimercapto-1,3-thiaselenole-2-thionato(2−)-S^4,S^5] zincate(2−)



M 551.9 (ion)

Bis-tetrabutylammonium salt: [130726-29-3].
Dark red cryst. (MeOH). Dec. at 150-153°.

Olk, R.-M. *et al, Z. Anorg. Allg. Chem.*, 1990, **581**, 59 (*synth, ir, cmr, uv*)

$C_6S_{10}Zn^{2\ominus}$ IC-005674

Bis[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-S^4,S^5] zincate(2−), 9CI

[55032-98-9]

As Bis[4,5-dimercapto-1,3-dithiole-2-onato(2−)-S^4,S^5] zincate(2−), IC-005646 with

X = Y = S

M 458.1 (ion)
Approx. tetrahedral at Zn.

Bis-tetrabutylammonium salt: [68449-38-7].
Wine-red cryst. Sol. Me_2CO. Mp 172-173°.
1,1-Dimethyl-4,4′-bipyridinium(2+) salt: [107769-58-4].
Dark green needles. Mp 245°.

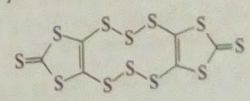
Steimecke, G. *et al, Z. Chem.*, 1975, **15**, 28 (*synth, elect prop*)
Fernandez, A. *et al, Chem. Ber.*, 1984, **117**, 3102 (*photochem, photophys*)
Wang, H. *et al, Wuli Huaxue Xuebao*, 1985, **1**, 378 (*cryst struct*)
Lahner, S. *et al, Chem. Ber.*, 1987, **120**, 1011 (*synth, uv-vis*)
Olk, R.M. *et al, Z. Anorg. Allg. Chem.*, 1988, **567**, 131 (*synth, cmr, ir*)

IC-005675

C_6S_{12}

Bis[1,3]dithiolo[4,5-*d*:4′5′-*i*][1,2,3,6,7,8]hexathiecin-2,8-dithione, 9CI

[120385-41-3]



M 456.8

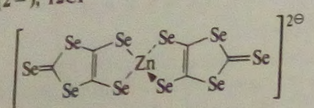
Orange prisms. Insol. all solvents tested.

Yang, X. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 3465 (*synth, ir, ms, cryst struct*)

IC-005676

$C_6Se_{10}Zn^{2\ominus}$

Bis[4,5-diselenyl-1,3-diselenole-2-selonato(2−)-Se^4,Se^5] zincate(2−), 12CI



M 927.0 (ion)

Bis-Ph_4As salt: [94509-37-2].
Dark red cryst. Mp 146-148° dec.

Olk, R.-M. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **544**, 199 (*synth*)

IC-005677

$C_7AsF_6MnO_5$

[Bis(trifluoromethyl)arsino]pentacarbonylmanganese, 9CI

[55997-37-0]

$(F_3C)_2AsMn(CO)_5$

M 407.9
Synth. from $HMn(CO)_5$ and $(CF_3)_2AsAs(CF_3)_2$. Viscous orange-yellow oil. Ir ν_{CO} 2124m, 2067w, 2038vs, 2021s cm^{-1}.

Grobe, J. *et al*, *Z. Anorg. Allg. Chem.*, 1975, **414**, 19 (*synth, F-19 nmr, ir*)
Demuth, R. *et al*, *Z. Naturforsch., B*, 1975, **30**, 539 (*ir, raman*)
Grobe, J. *et al*, *J. Fluorine Chem.*, 1978, **11**, 265 (*synth, ir, F-19 nmr*)

IC-005678

$C_7ErN_7S_7^{4\ominus}$

Heptakis(thiocyanato-*N*)erbate(*III*)(4−)
Heptaisothiocyanatoerbate(4−)

$[Er(NCS)_7]^{4\ominus}$

M 573.8 (ion)
7-Coord. Similar ions formed by Dy, Yb.

Tetrakis-Me_4N salt: [117074-74-5].
Pink cryst. Pentagonal bipyramidal Eu.

Tetrakis-Et_4N salt: [117673-88-8].
Pink cryst. + H_2O. Sol. MeOH. 8-Coord. struct. (H_2O coord.). Similar compds. obtd. for La, Ce, Pr, Nd, Dy.

Tateyama, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 2805.
Matsumura, N. *et al*, *Kidorui*, 1988, **12**, 146; *CA*, **109**, 182420 (*synth, cryst struct*)

IC-005679

$C_7F_3MnO_7$

Pentacarbonyl(trifluoroacetato)manganese(*I*), 11CI
Trifluoroacetato-O-pentacarbonylmanganese(I)

[15219-49-5]

$Mn(CO)_5(OOCCF_3)$

M 308.0
Mn—O 203.1 pm; two CO may be displaced by donor ligands e.g. Py, PPh_3. Synth. from $MnCl(CO)_5$ and $AgOOCCF_3$ or $Mn(\eta^1\text{-}C_3H_3)(CO)_5$ and F_3CCOOH. Volatile yellow cryst. (CH_2Cl_2/hexane). Mp °ca.71.

Green, M.L.H. *et al*, *J. Organomet. Chem.*, 1967, **8**, 511 (*synth*)
King, R.B. *et al*, *J. Organomet. Chem.*, 1968, **15**, 457 (*synth, ir, F-19 nmr*)
King, R.B. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 2169 (*props*)
Garner, C.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 735 (*synth, F-19 nmr, ir, raman, pe, ms, reactions*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1981, **20**, 1287 (*cryst struct*)

IC-005680

$C_7F_5MnO_5$

Pentacarbonyl(pentafluoroethyl)manganese, 8CI

[20791-80-4]

$Mn(CF_2CF_3)(CO)_5$ (O_h)

M 314.0
Low-melting air-stable v. volatile white cryst. or liq. Mp 15-17°. Bp 155° (extrap.). Ir ν_{CO} 2130w, 2072w, 2038vs, 2023s, 2002w, 1983vw cm^{-1} (C_2Cl_4).

Kaesz, H.D. *et al*, *Z. Naturforsch., B*, 1960, **15**, 763 (*synth, props*)
Pitcher, E. *et al*, *J. Chem. Phys.*, 1962, **36**, 124 (*F-19 nmr*)
Pitcher, E. *et al*, *Spectrochim. Acta*, 1962, **18**, 585 (*ir*)

IC-005681

$C_7F_6MnO_5P$

[Bis(trifluoromethyl)phosphino]pentacarbonylmanganese, 9CI

[56112-22-2]

$(F_3C)_2PMn(CO)_5$

M 363.9
Synth. from $HMn(CO)_5$ and $(CF_3)_2P{-}P(CF_3)_2$. Yellow oil. Ir ν_{CO} 2129m, 2073w, 2045vs, 2023s cm^{-1}.

Grobe, J. *et al*, *Z. Anorg. Allg. Chem.*, 1975, **414**, 19 (*synth, F-19 nmr, ir*)
Demuth, R. *et al*, *Z. Naturforsch., B*, 1975, **30**, 539 (*ir, raman*)
Grobe, J. *et al*, *J. Fluorine Chem.*, 1978, **11**, 265 (*synth, ir, F-19 nmr*)

IC-005682

$C_7F_6N_2O_6ReS^{\ominus}$

Pentacarbonyl[1,1,1-trifluoro-*N*-(thiazyloxy)-*N*-(trifluoromethyl)methanamine-$N^{\wedge}$]rhenium(1+), 11CI

$[(OC)_5ReN{=}SO{-}N(CF_3)_2]^{\ominus}$

M 540.3 (ion)

Hexafluoroarsenate: Bright-red cryst. Dec. at 135°.

Hartmann, G. *et al*, *J. Organomet. Chem.*, 1983, **252**, 195 (*synth, ir*)

IC-005683

$C_7FeMnNO_8^{2\ominus}$

Tricarbonylnitrosyl(tetracarbonylferrate)manganate(2−), 11CI

$[(OC)_4Fe{-}Mn(CO)_3NO]^{2\ominus}$

M 336.8 (ion)

Bis[bis(triphenylphosphine)iminium] salt: [84928-65-4].
Synth. from $K_2[Mn(NO)(CO)_4]$ and $Fe(CO)_5$ in THF followed by addition of $[(Ph_3P)_2N]Cl$. Golden microcryst. (THF). Ir ν_{CO} 1985m, 1940w, 1870s; ν_{NO} 1645m cm^{-1} (THF).

Chen, Y.-S. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 1689 (*synth, ir, pmr*)

IC-005684

$C_7H_3CrNO_5S$

Pentacarbonyl(methyl thiocyanate-*N*)chromium, 10CI

[57196-01-7]

$(OC)_5CrNCSMe$

M 265.1

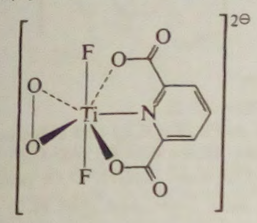
Yellow cryst. (hexane). Sol. org. solvs., esp. THF, Me_2CO. Mp 39-41° dec. Dec. in several hours in air at r.t. but indefinitely stable at 0° in an inert atm. in the dark. Ir ν_{CN} 2176 cm^{-1} (pentane).

Quick, M.H. *et al*, *Inorg. Chem.*, 1976, **15**, 160 (*synth, ir, pmr*)
Goddard, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1255 (*synth, cryst struct*)

IC-005685

$C_7H_3F_2NO_6Ti^{2\ominus}$

Difluoroperoxy[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6] titanate(*IV*)(2−), 9CI
Difluoroperoxo(dipicolinato)titanate(IV)(2−)



M 282.9 (ion)
Approx. pentagonal bipyramid. The neutral compd. $[Ti(O_2)$dipicolinate$(H_2O)_2]$ has a similar struct. in which H_2O replaces $F^{\ominus}$. This compd. is red suggesting some difference in bonding of the peroxy group.

Di-K salt: [41077-36-5].
Synth. by reaction of $TiCl_4$ with H_2O_2 at low temps., adding dipicolinic acid and adjusting with KOH to pH5. Red-orange cryst. $+2H_2O$.

Mühlebach, J. *et al*, *Inorg. Chem.*, 1970, **9**, 2381 (*synth*)
Schwarzenbach, D., *Helv. Chim. Acta*, 1972, **55**, 2990 (*cryst struct*)

IC-005686

$C_7H_3MnNO_5^{\ominus}$

(Acetonitrile)pentacarbonylmanganese(1+), 9CI
Pentacarbonylacetonitrilemanganese(1+).
Pentacarbonyl(cyanomethane)manganese(1+)

[27674-37-9]

$[Mn(CO)_5(NCMe)]^{\ominus}$

M 236.0 (ion)
Synth. by a variety of methods including reaction of $Mn(OClO_3)(CO)_5$ or $Mn(O_3SCF_3)(CO)_5$ with MeCN and $MnBr(CO)_5$ and $[NO]PF_6$ in MeCN.

Hexafluorophosphate: [37504-44-2].
Air-stable white cryst. (Me_2CO/Et_2O). Sol. polar solvs., solns. unstable to air. Ir ν_{CO} 2140w, 2061vs, 2043sh cm^{-1} (Me_2CO).

Tetrafluoroborate: [75008-28-5].
Pale-yellow or colourless cryst. (MeCN/Et_2O). Ir ν_{CO} 2140w, 2060s, 2045sh cm^{-1}.

Connelly, N.G. *et al*, *J. Organomet. Chem.*, 1972, **38**, 385 (*synth, ir*)
Drew, D. *et al*, *Inorg. Chem.*, 1975, **14**, 1579 (*synth*)
Darensbourg, D.J. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 4726, 5940 (*synth, props*)
Wimmer, F.L. *et al*, *Aust. J. Chem.*, 1978, **31**, 267 (*synth*)
Trogler, W.C., *J. Am. Chem. Soc.*, 1979, **101**, 6459 (*synth, props*)
Snow, M.R. *et al*, *Inorg. Chim. Acta*, 1980, **44**, L189 (*synth*)
Raab, K. *et al*, *Z. Naturforsch., B*, 1983, **38**, 1466 (*synth, ir, pmr*)

IC-005687

$C_7H_3MnNO_5^{\ominus}$

Pentacarbonyl(isocyanomethane)manganese(1+), 9CI
Pentacarbonyl(methyl isocyanide)manganese(1+)

[45113-87-9]

$[Mn(CO)_5(CNMe)]^{\ominus}$ (C_{4v})

M 236.0 (ion)
Hexafluorophosphate: [38979-19-0].
Synth. from $MnBr(CO)_4(CNMe)$, $AlCl_3$ and CO followed by addition of NH_4PF_6. Cryst. (Me_2CO/Et_2O). Mp 192-194°. Ir ν_{CO} 2158, 2075; ν_{CN} 2264 cm^{-1}.

Treichel, P.M. *et al*, *J. Organomet. Chem.*, 1972, **44**, 339 (*synth, ir, pmr, props*)
Sarapu, A. *et al*, *Inorg. Chem.*, 1975, **14**, 247 (*synth, props*)

IC-005688

$C_7H_3NO_5Re^{\ominus}$

(Acetonitrile)pentacarbonylrhenium(1+)

[29421-17-8]

$[H_3CCNRe(CO)_5]^{\ominus}$ (C_{4v})

M 367.3 (ion)
Hexafluorophosphate: [55057-83-5].
$NOPF_6$, $Re_2(CO)_{10}$ and MeCN. Off-white powder; air-stable as solid, but air-sensitive in soln. Sol. polar solvs. Mp 163-170°. Ir ν_{CO} 2159w, 2050vs, 2021sh, cm^{-1} (Me_2CO).

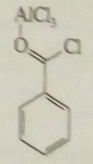
Connelly, N.G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 880 (*synth, ir*)
Drew, D. *et al*, *Inorg. Chem.*, 1975, **14**, 1579 (*synth, ir*)

IC-005689

$C_7H_5AlCl_4O$

(Benzoyl chloride)trichloroaluminium
Benzoyl chloride compd. with aluminium chloride (1:1)

[36525-11-8]



M 273.9
Colourless moisture-sensitive cryst. (CS_2). Mp 93°. Species in soln. may be complex.

[14854-48-9]

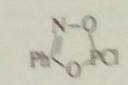
Rasmussen, S.E. *et al*, *Acta Chem. Scand.*, 1966, **20**, 1351 (*synth, cryst struct*)
Corriu, R. *et al*, *Tetrahedron*, 1971, **27**, 5801 (*ir, use*)

IC-005690

$C_7H_5ClNO_2P$

2-Chloro-5-phenyl-1,3,4,2-dioxazaphosphole, 10CI
Benzhydroxamatophosphorus(III) chloride

[66181-07-5]



M 201.5
V. hygroscopic pungent liq. $Bp_{0.05}$ 45° (bath 75°). Easily hydrol.

▷ Explodes at bath temp. 90°.

2-Oxide: [66181-06-4].
$C_7H_5ClNO_3P$ M 217.5
Liq. $Bp_{0.001}$ 84-86°.

2,2-Dichloro-2,2-dihydro- [66181-02-0]. *2,2,2-Trichloro-2,2-dihydro-5-phenyl-1,3,4,2-dioxazaphosphole*
$C_8H_6Cl_2NO_2P$ M 272.4
V. hygroscopic liq. $Bp_{0.001}$ 90°.

Fluck, E. *et al*, *Z. Anorg. Allg. Chem.*, 1977, **437**, 53 (*synth, derivs, P-31 nmr*)
Von Hinrichs, E. *et al*, *J. Chem. Res. (S)*, 1978, 338 (*synth, derivs, P-31 nmr*)
Burilov, A.R. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1986, 945; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1986, 862 (*synth, reactions, P-31 nmr*)

$C_7H_4Cl_3IrNO_4^{3\ominus}$ IC-005691

Trichlorooxalato(pyridine)iridate(*II*)(3−)

$[Ir(C_2O_4)(Py)Cl_3]^{3\ominus}$

M 465.6 (ion)
Unusual example of stable Ir(*II*), if formulation correct.
Tri-K salt: Deep orange solid. Sol. H_2O.

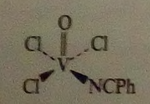
Inamura, Y., *Bull. Soc. Chem. Fr.*, 1940, **7**, 750 (*synth*)
Mathieu, J.P. *et al*, *J. Chem. Phys.*, 1962, **59**, 369 (*synth*)

$C_7H_4Cl_3NOV$ IC-005692

(Benzonitrile)trichlorooxovanadium(*V*), 10Cl

Oxotrichloro(benzonitrile)vanadium(V). *Vanadium*(V) *oxychloride benzonitrile*

[73164-98-4]



M 276.4
Square pyramidal. Synth. by dissolving $VOCl_3$ in PhCN. Black solid. The nitrile dissociates reversibly on heating *in vacuo*. See also (Benzeneacetonitrile) trichlorooxovanadium(*V*), IC-005918 and Bis(benzonitrile)trichlorooxovanadium(*V*), IC-008530.

Gourdon, A. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 304 (*synth, cryst struct*)

$C_7H_5Cl_3O_2Ti$ IC-005693

(Benzoato-*O*)trichlorotitanium(*IV*), 11Cl

[27905-52-8]

$PhCOOTiCl_3$

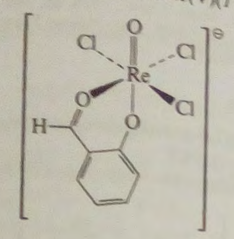
M 275.3
Tetrahedral. Synth. by reaction of $TiCl_4$ and benzoic acid in C_6H_6 soln. Component of olefin polym. catalysts; also catalyses anomerisation of carbohydrates. White solid which hydrol. in EtOAc to $Ti_2(\mu\text{-}O)(\mu\text{-benzoato})_2Cl_4(EtOAc)_2$.

Varma, I.D. *et al*, *J. Prakt. Chem.*, 1959, **8**, 64 (*synth*)
Japan. Pat., 74 38 030, (1974); *CA*, **82**, 126374m (*use*)
Ger. Pat., 2 612 650, (1976); *CA*, **86**, 17316f (*use*)
Csuros, Z. *et al*, *Carbohydr. Res.*, 1980, **82**, 273 (*use*)
Veneditkova, N.A. *et al*, *Vysokomol. Soedin., Ser. A*, 1985, **27**, 1452; *CA*, **104**, 6207k (*rev, olefin polym*)
Alcock, N.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 614 (*hydrol*)

$C_7H_5Cl_3O_3Re^{\ominus}$ IC-005694

Trichloro(2-hydroxybenzaldehydato-*O,O'*)oxorhenate(*V*) (1−), 11Cl

Trichlorooxo(salicylato-O,O')rhenate(V)(1−)



M 429.6 (ion)
Ir $\nu_{Re=O}$ 960 cm^{-1}.
Ph_4As salt: [89164-43-2].
Synth. from $AsPh_4[ReOCl_4]$ and salicylic acid in boiling EtOH. Yellow brown powder (Me_2CO). Sol. CH_2Cl_2, $CHCl_3$, Me_2CO; insol. EtOH, Et_2O, pentane. Mp 219°.

Duatti, A. *et al*, *Inorg. Chim. Acta*, 1984, **81**, 21 (*synth, ir, props*)

$C_7H_5Cl_5O_2Ti^{2\ominus}$ IC-005695

(Benzoato-*O*)pentachlorotitanate(*IV*)(2−), 11Cl

$[PhCOOTiCl_5]^{2\ominus}$

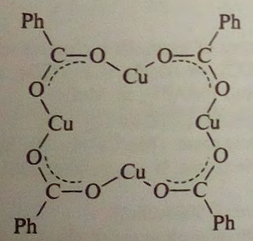
M 346.2 (ion)
This is one of a number of salts $(MgL_x)TiCl_5L'$. All are active olefin polym. catalysts.
Bis(ethyl acetate-O)magnesium salt: [93855-89-1].
$C_{15}H_{21}Cl_5MgO_6Ti$ M 546.7
Synth. by dissolving $TiCl_4$, $MgCl_2$ and benzoic acid in EtOAc. Yellow solid.

Albizzati, E. *et al*, *Makromol. Chem. Rapid Commun.*, 1985, **5**, 673 (*synth, use*)

$C_7H_5CuO_2$ IC-005696

Copper(*I*) benzoate

Benzoatocopper



tetramer

M 184.6
Tetrameric struct. in solid state. Source of doubly bridged dimetallic unit in reaction with many substrates. Binds isocyanides. In presence of amines, binds CO to afford isolable complexes; alone, CO binds reversibly.
p-*Tolylisocyanide complex (dimeric):* see *Bis[μ-(benzoato-O:O')]bis(1-isocyano-4-methylbenzene)dicopper*(I), *12Cl, IC-012378*
Tetramer: [62914-01-6]. ***Tetrakis[μ-(benzoato-O:O')] tetracopper*(I)**
$C_{28}H_{20}Cu_4O_8$ M 738.6
Cryst.

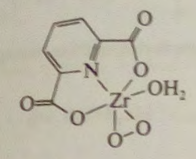
Edwards, D.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2463 (*synth*)

Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 299 (*cryst struct*)
Pasquali, M. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 4092 (*reactions*)
Doyle, G. *et al*, *Organometallics*, 1982, **1**, 1613 (*synth, reactions*)
Toth, A. *et al*, *Inorg. Chem.*, 1987, **26**, 236 (*use*)

$C_7H_5NO_7Zr$ IC-005697

Aquaperoxy[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6] zirconium(*IV*), 11Cl

[102149-90-6]



M 306.3
Config. around Zr not specified. Synth. by adding $Zr(NO_3)_4.4H_2O$ in 30% H_2O_2 to Me_2CO soln. of 2,6-pyridinecarboxylic acid. White solid. Sol. MeOH, DMSO, $MeNO_2$; insol. H_2O, hexane.

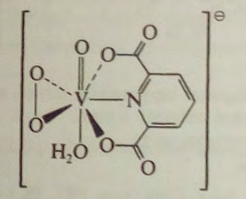
Tarafder, M.T.H. *et al*, *Inorg. Chem.*, 1986, **25**, 2265 (*synth, ir, cmr*)

$C_7H_5NO_8V^{\ominus}$ IC-005698

Aquaoxoperoxy[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6] vanadate(*V*)(1−), 11Cl

Aquaoxoperoxy(dipicolinato)vanadate(V)(1−)

[62126-18-5]



M 282.0 (ion)
Pentagonal bipyramid with O and H_2O in axial sites.
K salt: [64440-67-1].
Synth. by dissolving V_2O_5 and picolinic acid in H_2O adding 30% H_2O_2 then saturated KCl soln. Red-orange solid.
NH_4 salt: [40633-57-6].
Synth. from NH_4VO_3, picolinic acid and H_2O_2 in H_2O. Dark red solid + variable H_2O.
Ph_4P salt: [89772-74-7].
Epoxidation reagent for olefins and hydroxylation of hydrocarbons.

[80040-87-5]

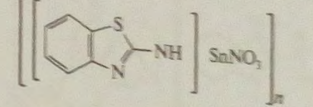
Drew, R.E. *et al*, *Inorg. Chem.*, 1973, **12**, 829 (*synth, cryst struct, NH_4 salt*)
Wieghardt, K., *Inorg. Chem.*, 1978, **17**, 57 (*synth, K salt*)
Rehder, D. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1251 (*V-51 nmr, K salt*)
Eur. Pat., 97 551, (1984); *CA*, **100**, 174641h (*reaction, use*)

$C_7H_5N_3O_3SSn$ IC-005699

(2-Aminobenzothiazolato)nitratotin(*II*)

(2-Benzothiazolaminato-N^3)(nitrato-O)tin, 9Cl

[57107-27-4]

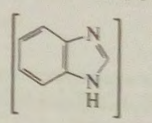


M 329.9
Polymeric with bridging nitrate groups and organic ligands. Synth. from $Ph_2Sn(NO_3)_2$ and 2-aminobenzothiazole in Me_2CO. White tabular cryst.

Nardelli, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1595 (*synth, cryst struct*)

$C_7H_6Cl_2N_2Ni$ IC-005700

(Benzimidazole)dichloronickel(*II*)



M 247.7
Octahedral at Ni with bridging Cl. Yellow solid. μ_{eff} = 3.31 μ_B.

Goodgame, D.M.L. *et al*, *J. Chem. Soc.*, 1964, 5194 (*synth, uv-vis, magnetism*)

$C_7H_6Cl_4MoN_2O_3Sn$ IC-005701

Bis(acetonitrile)tricarbonylchloro(trichlorostannyl) molybdenum(*II*)

[120254-22-0]

$MoCl(SnCl_3)(CO)_3(NCMe)_2$

M 522.5
Air-sensitive orange cryst. (MeCN). Ir $\nu_{N\equiv C}$ 2288, 2258; ν_{CO} 2026, 1939, 1912 cm^{-1}.

Baker, P.K. *et al*, *J. Organomet. Chem.*, 1989, **359**, 189 (*synth*)

$C_7H_6CrN_2O_5S$ IC-005702

Pentacarbonyl(1,1-dimethylthionitrosamine)chromium

Pentacarbonyl[N-*methyl*-N-(*thionitroso*)*methanamine*-S] *chromium, 11Cl*

[78230-48-5]

$Me_2NNSCr(CO)_5$

M 282.1
Ruby red cryst. Sol. CH_2Cl_2. Mp 110° dec. Ir 2000m, 1945vs, 1890vs, 1360s, 1260m, 1120m, 1090m, 1020m, 800m, 785m cm^{-1}.

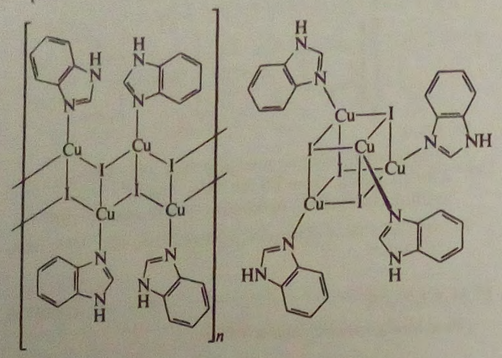
Roesky, H.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 183 (*synth, cryst struct, pmr, ir, ms*)

IC-005703

$C_7H_6CuIN_2$

(1*H*-Benzimidazole-N^3)iodocopper(*I*), 12CI

[52155-37-0]



step polymer *tetramer*

M 308.5

Known in solid state as step-polymer or tetrameric forms.

Step polymer: catena-(μ_3-*Iodo*)(*benzimidazole*)*copper*(I)
White solid or colourless cryst.

Tetramer: [110682-65-0]. *Tetrakis*(*1H-benzimidazole*-N^3)*tetra*-μ_3-*iodotetracopper*(I), *12CI*

$C_{28}H_{24}Cu_4I_4N_8$ M 1234.3

Colourless cryst. + 3 diglyme. Sol. diglyme; insol. MeOH.

Toth, A. *et al*, *Inorg. Chem.*, 1987, **26**, 3897 (*synth*, *cryst struct*)

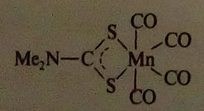
IC-005704

$C_7H_6MnNO_4S_2$

Tetracarbonyl(*N*,*N*-dimethyldithiocarbamato)manganese

Tetracarbonyl(*dimethylcarbamodithioato*-S,S′)*manganese*, *9CI*

[39142-22-8]



M 287.1

Synth. from $MnBr(CO)_5$ and $Me_3SnS_2CNMe_2$. Volatile yellow or orange-red cryst. Mp 71° dec. $Subl._{0.01}$ 50°. Ir ν_{CO} 2087, 2008, 1994, 1956 cm^{-1}.

Abel, E.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 98 (*synth*, *ir*, *pmr*, *ms*)

Tanaka, K. *et al*, *Inorg. Chem.*, 1975, **14**, 1545 (*synth*, *ir*)

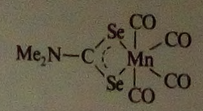
IC-005705

$C_7H_6MnNO_4Se_2$

Tetracarbonyl(*N*,*N*-dimethyldiselenocarbamato)manganese

Tetracarbonyl(*dimethylcarbamodiselenoato*-Se,Se′)*manganese*, *9CI*

[54751-23-4]



M 380.9

Synth. from $MnBr(CO)_5$ and $Me_2ClSnSe_2CNMe_2$. Yellow cryst. $Subl._{0.001}$ 50°. Dec. at 85°.

Tanaka, K. *et al*, *Inorg. Chem.*, 1975, **14**, 1545 (*synth*, *ir*)

$C_7H_6MnNO_5$

(Dimethylamino)pentacarbonylmanganese IC-005706

$Me_2NMn(CO)_5$

M 239.0

Synth. from Me_3SnNMe_2 and $MnBr(CO)_5$. No phys. props. reported.

George, T.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 463 (*synth*)

$C_7H_6MnO_5P$

Pentacarbonyl(dimethylphosphino)manganese, 10CI IC-005707

[66672-66-0]

$Me_2PMn(CO)_5$

M 256.0

Synth. from Me_2PPMe_2 and $HMn(CO)_5$. Yellow oil.

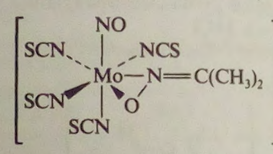
Grobe, J. *et al*, *J. Fluorine Chem.*, 1978, **11**, 265 (*synth*, *ms*)

IC-005708

$C_7H_6MoN_6O_2S_4^{2\ominus}$

Nitrosyl(2-propanone oximato-*N*,*O*)tetrakis(thiocyanato-*N*)molybdate(2−), 10CI

Isopropyloximato-N,O-*tetrakis*(*isothiocyanato*)*nitrosylmolybdate*(2−). (*Acetoneoximato*-N,O)*tetrakis*(*isothiocyanato*)*nitrosylmolybdate*(2−)



M 430.3 (ion)

Distorted pentagonal bipyramidal struct. with unusual side-on bonded oximato ligand.

Bis-Ph_4P salt: [77438-30-3].
Yellow cryst.

Muller, A. *et al*, *Inorg. Chim. Acta*, 1981, **55**, L33 (*cryst struct*, *synth*)

Muller, A. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **480**, 157 (*cryst struct*, *synth*)

IC-005709

$C_7H_6N_2O_5Pb$

(4-Aminobenzoato)(nitrato)lead(*II*)

[71652-10-3]

$[Pb(H_2NC_6H_4COO)NO_3]_n$

M 405.3

Polymeric struct. consists of Pb(*II*) and $COO^{\ominus}$ (from ligand) chains. Synth. from 0.01*M* hot aq. solns. of $Pb(NO_3)_2$ and $H_2NC_6H_4COONa$. Pale yellow triclinic cryst.

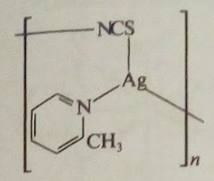
Amiraslanov, I.R. *et al*, *Zh. Strukt. Khim.*, 1980, **21**, 137; *Russ. J. Struct. Chem.* (*Engl. Transl.*), 1980, **21**, 109 (*synth*, *cryst struct*)

IC-005710

$C_7H_7AgN_2S$

(2-Methylpyridine)(thiocyanato-*S*)silver(*I*), 11CI

[89413-37-6]



M 259.0

Infinite polymer with trigonal Ag and bridging NCS. Cryst.

Mills, N.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 229 (*cryst struct*)

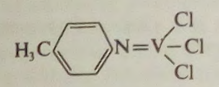
IC-005711

$C_7H_7Cl_3NV$

Trichloro(*p*-tolylimido)vanadium

Trichloro[*4-methylbenzenaminato*(2−)]*vanadium*, *11CI*

[90941-76-7]



M 262.4

Synth. by reaction of a soln. of *p*-tolyl isocyanate in octane with a soln. of $VOCl_3$ in the same solvent. Purple-black cryst. by subl. Sol. THF, CH_2Cl_2. $Subl._{0.0001}$ 130°. Forms 1:1 adducts with several donors. Thermally stable but v. moisture-sensitive.

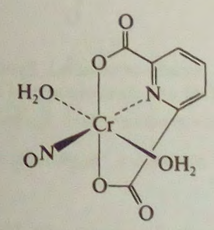
Maatta, E.A., *Inorg. Chem.*, 1984, **23**, 2560 (*synth*, *pmr*, *ms*, *V-51 nmr*)

IC-005712

$C_7H_7CrN_2O_7$

Diaquanitrosyl[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6]chromium, 11CI

[94288-72-9]



M 283.1

mer, *trans*-Octahedral with Cr—NO 169.9, N—O 118.2 pm; angle: CrNO 180°. Synth. by reduction of $CrO_4^{2\ominus}$ with $NH_2OH.HCl$ in presence of ligand. Red cryst. Ir ν_{NO} 1725 cm^{-1}; $\mu_{eff} = 1.70\mu_B$ (298K).

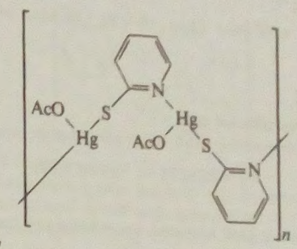
Wieghardt, K. *et al*, *Inorg. Chim. Acta*, 1984, **89**, L43 (*cryst struct*, *synth*)

$C_7H_7HgNO_2S$

(Acetato-*O*)(2(1*H*)-pyridinethionato-*S*)mercury IC-005713

(*Acetato*-O)(*2-pyridinethiolato*)*mercury*

[121176-08-7]



M 369.7

1-D polymer in solid state. Near-neighbour interactions → approx. octahedral Hg. Cryst. (CH_2Cl_2/Et_2O). Mp 175°.

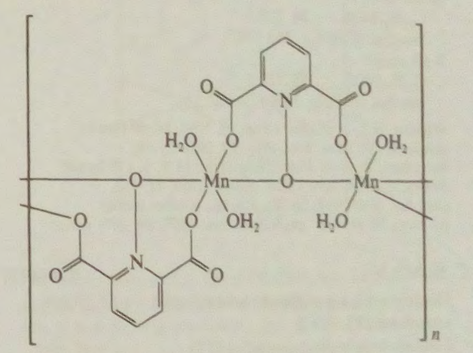
Wang, S. *et al*, *Inorg. Chem.*, 1989, **28**, 2615 (*synth*, *pmr*, *ir*, *cryst struct*)

$C_7H_7MnNO_7$

Diaqua[2,6-pyridinedicarboxylic acid 1-oxidato(2−)-O^1,O^2]manganese(*II*), 11CI IC-005714

Diaqua(*pyridine-2,6-dicarboxylate*-N-*oxido*)*manganese*(II)

[97277-46-8]



M 272.0

Polymeric chain struct. with approx. octahedral high spin Mn(*II*). Synth. from $Mn(OAc)_2.4H_2O$ and pyridine-2,6-dicarboxylic acid in H_2O. Yellow cryst. (H_2O). Insol. H_2O. Mp 257-263° dec. $\mu_{eff} = 5.88\mu_B$ per Mn.

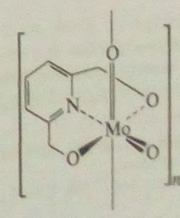
Nathan, L.C. *et al*, *Inorg. Chem.*, 1985, **24**, 2763 (*synth*, *cryst struct*, *magnetism*, *ir*, *esr*, *uv*)

IC-005715

$C_7H_7MoNO_4$

Dioxo[2,6-pyridinedimethanolato(2−)-N,O^a,O^a]molybdenum(*VI*), 11CI

[85534-02-7]



M 265.0

Pseudo-octahedral Mo in polymeric chain struct. with Mo=O 171.0, 171.9 pm. Synth. from $MoO_2(acac)_2$ + L-NO_2 (MeOH). Model for Mo containing enzymes. Colourless cryst. (tetramethylene sulfoxide). Ir ν_{MoO} 909, 850 cm^{-1}.

Berg, J.M. *et al*, *Inorg. Chem.*, 1983, **22**, 1768 (*cryst struct, synth, ir*)

C_7H_7NOS IC-005716

Phenylthiocarbamic acid

Phenylcarbamothioic acid, 9CI. Thiocarbanilic acid

PhNHCSOH ⇌ PhNHCOSH

M 153.2

O-Alkyl esters have acaridial, anaesthetic and fungistatic activity.

Ag salt:
C_7H_6AgNOS M 260.0
Bronze-yellow cryst. ($CHCl_3$/EtOH). Mp 186°.

O-Me ester: [13509-41-6].
C_8H_9NOS M 167.2
Bactericide. Cryst. (EtOH). Mp 97°.

S-Me ester: [13509-38-1].
C_8H_9NOS M 167.2
Leaflets (EtOH aq.). Mp 83-84°.
▷ FD9787000.

O-Ph ester:
$C_{13}H_{11}NOS$ M 229.3
Needles ($CHCl_3$). Mp 142°.

S-Ph ester:
$C_{13}H_{11}NOS$ M 229.3
Needles (EtOH). Mp 122-122.5°.

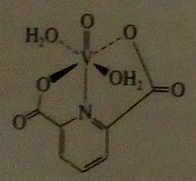
Wheeler, H.L. *et al*, *Am. Chem. J.*, 1900, **24**, 60 (*synth*)
Schneider, W. *et al*, *Ber.*, 1914, **47**, 2038 (*synth*)
Bettschart, A. *et al*, *Helv. Chim. Acta*, 1919, **2**, 118 (*synth*)
Svátek, E. *et al*, *Acta Chem. Scand.*, 1959, **13**, 442.
Ger. Pat., 2 617 917, (1976); *CA*, **86**, 43426m (*synth*)
Al-Rawi, H. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 2671 (*struct*)

$C_7H_7NO_7V$ IC-005717

Diaquaoxo[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6]vanadium(*IV*), 11CI

Diaquaoxodipicolinatovanadium(IV)

[18582-04-2]



M 268.0
Octahedral.

Monohydrate: [17442-64-7].
Deep blue solid.

Dihydrate: [21361-01-3].
Synth. by the action of the free acid on an aq. slurry of freshly prepared vanadyl hydroxide. Green solid (H_2O at pH <1.8). Paramagnetic; μ_{eff} = 1.69 μ_B (r.t.).

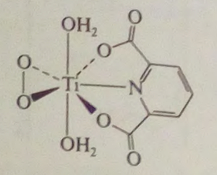
[32354-74-8]

Dutta, R.L. *et al*, *J. Indian Chem. Soc.*, 1967, **44**, 273 (*synth, uv-vis, magnetism, monohydrate*)
Bersted, B.H. *et al*, *Inorg. Chem.*, 1968, **7**, 1557 (*synth, cryst struct, dihydrate*)
Funahashi, S. *et al*, *Inorg. Chem.*, 1982, **21**, 2202 (*reaction*)

$C_7H_7NO_8Ti$ IC-005718

Diaquaperoxy[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6]titanium(*IV*), 9CI

Diaquaperoxo(dipicolinato)titanium(IV)



M 281.0
Pentagonal bipyramid. Synth. from soln. of $TiCl_4$ in conc. H_2O_2 and ligand at controlled pH. Deep red triclinic or orthorhombic cryst., the triclinic form is pleochroic but the geometry of the complex ion is unaltered in both modifications. Sol. H_2O.

Dihydrate: [30138-15-9].
[41189-90-6]

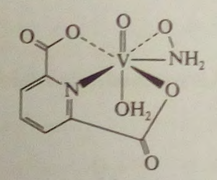
Schwarzenbach, G. *et al*, *Inorg. Chem.*, 1970, **9**, 2381 (*synth*)
Schwarzenbach, D., *Helv. Chim. Acta*, 1972, **55**, 2990 (*cryst struct, triclinic form*)
Manohar, H. *et al*, *Helv. Chim. Acta*, 1974, **57**, 1086 (*cryst struct, orthorhombic form*)

$C_7H_7N_2O_7V$ IC-005719

Aqua(hydroxyaminato)oxo(pyridine-2,6-dicarboxylato)vanadium(*V*)

Aquaoxo(hydroxylaminato)(dipicolinato)vanadium(V).
*Aqua(hydroxylaminato-*N,O*)oxo[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6]vanadium*(V), *11CI*

[77489-73-7]



M 282.0
7-Coordinate but pseudo-octahedral. Synth. from NH_4VO_3, NH_2OH and dipicolinic acid in H_2O. Cryst.

Nuber, B. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 947 (*cryst struct*)
Rehder, D. *et al*, *Z. Naturforsch., B*, 1981, **36**, 1251 (*synth, V-51 nmr*)

$C_7H_8MnN_3O_3S$ IC-005720

(Methylthiobenzene)trinitrosylmanganese, 11CI

(Methyl phenyl sulfide)trinitrosylmanganese

[97867-13-5]

$Mn(NO)_3SMePh$

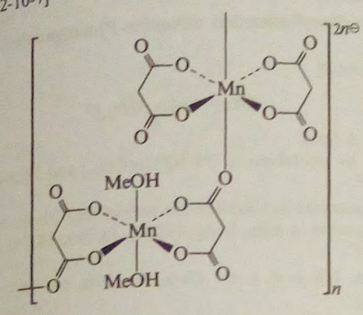
M 269.1
Synth. from $Mn(NO)_3THF$ in pentane with PhSMe.

Rehder, D. *et al*, *Inorg. Chim. Acta*, 1985, **100**, L11 (*synth, Mn-55 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 80 (*rev, bibl*)

$C_7H_8MnO_9^{\ominus}$ IC-005721

Methanolbis[propanedioato(2−)-*O*,*O*′]manganate(*III*) (1−), 10CI

[22572-10-7]



dimeric anion

M 291.0 (ion)
trans-Octahedral Mn in carboxylate bridged polymeric chain struct. of alternating $[Mn(MeOH)_2(malonate)_2]^{\ominus}$ and $[Mn(malonate)_2]^{\ominus}$ anions.

K salt: Synth. from malonic acid in CH_2Cl_2, cyclohexanol and MeOH + $KMnO_4$. Air-stable green triclinic cryst. (CH_2Cl_2/cyclohexanol/MeOH). Previously formulated as $K[Mn(OH_2)_2(malonate)_2]$. μ_{eff} = 4.91 μ_B (300K); 4.29 μ_B (90K).

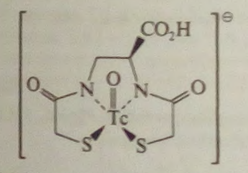
Lis, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 996 (*synth, cryst struct*)

$C_7H_8N_2O_5S_2Tc^{\ominus}$ IC-005722

[*N*,*N*′-Bis(mercaptoacetyl)-2,3-diaminopropanoato(4−)]oxotechnetate(*V*)(1−)

*[N-(Mercaptoacetyl)-3-[(mercaptoacetyl)amino]alaninato(5−)-*N,N′,S,S′*]oxotechnetate(2−), monohydrogen. [2,3-Bis(2-thioacetamido)propanoato]oxotechnetate*(V)(*1*−). *Tc-CO2-DADS. CO2-DADS-Tc*

[82795-08-2]



syn-form

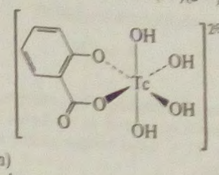
M 363.1 (ion)
Exists in *syn*- and *anti*- isomeric forms which can be separated chromatographically, but appear not to have been isolated as pure solid derivatives. Synth. from $TcO_4^{\ominus}$ plus ligand with $SnCl_2$, formamidine sulfinic acid, or $S_2O_4^{2\ominus}$ as reductant. Renal tubular function probe; *syn*-form more active than its isomer and shows better renal uptake and blood clearance than DADS parent compd.

Fritzberg, A.R. *et al*, *J. Nucl. Med.*, 1982, **23**, 592 (*synth, chromatog, pharmacokinetics*)
Costello, C.E. *et al*, *J. Nucl. Med.*, 1983, **24**, 353 (*pharmacokinetics*)
Kasina, S. *et al*, *J. Med. Chem.*, 1986, **29**, 1933 (*pharmacokinetics*)
Bubeck, B. *et al*, *Int. J. Rad. Appl. Instrum. [B]*, 1988, **15**, 99.

$C_7H_9O_7Tc^{2\ominus}$ IC-005723

Tetrahydroxy[2-hydroxybenzoato(2−)-*O*,*O*′]technetate(2−), 9CI

Tetrahydroxy(salicylato)technetate(IV)(2−)



M 303.0 (ion)
The Tc-salicylate system has been very little studied; the present compd. is not well-characterised.

Di-Tl(I) *salt:* [26195-56-2].
$C_7H_8O_7TcTl_2$ M 711.8

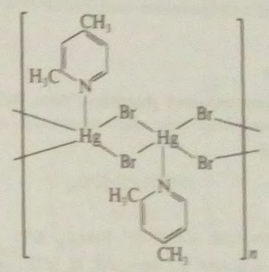
Ziolkowski, J. *et al*, *Theory Struct. Complex Compds., Papers Symp., 1964*, 419; *CA*, 1965, **63**, 17460e (*synth*)

$C_7H_9Br_2HgN$ IC-005724

Dibromo(2,4-dimethylpyridine)mercury

Dibromo(2,4-lutidine)mercury. (2,4-Lutidine)mercury dibromide

[28108-37-4]



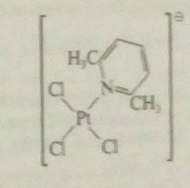
M 467.5
Polymeric chain struct. Cryst. (EtOH). Mp 142°.

Ahuja, I.S. *et al*, *J. Chem. Soc. A*, 1970, 2161 (*synth, ir*)
Bell, N.A. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 710 (*synth, cryst struct*)

$C_7H_9Cl_3NPt^{\ominus}$ IC-005725

Trichloro(2,6-dimethylpyridine)platinate(*II*)(1−), 9CI

Trichloro(2,6-lutidine)platinate(II)(*1*−)



M 408.5 (ion)
Square planar anion. Synth. from Tetrachloroplatinate(*II*) (2−), IC-017117 + 2,6-$Me_2C_6H_3N$.

K salt: [57407-61-1].
Yellow solid. Dec. at 230°.

Melanson, R. *et al*, *Can. J. Chem.*, 1976, **54**, 1002 (*cryst struct*)
Kong, P.-C. *et al*, *Can. J. Chem.*, 1978, **56**, 441 (*synth, ir, pmr*)

C_7H_9CuIN IC-005726

(2,4-Dimethylpyridine)iodocopper(*I*)

Poly[(2,4-dimethylpyridine)iodocopper], 12CI

[20631-74-7]

As Iodo(2-methylpyridine)copper(*I*), IC-004994 with

R = CH_3

M 297.6

Struct. based on edge-sharing Cu_2I_2 rhombs, with each Cu bound to three I and the N of the Lewis base. Synth. from CuI + KI + 2,4-dimethylpyridine in Me_2CO. White needles.

Rath, N.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 2449 (*synth, cryst struct*)

$C_7H_9FeO_4Sb$ IC-005727

Tetracarbonyl(trimethylstibine)iron, 9CI, 8CI

[30230-15-0]

$Me_3SbFe(CO)_4$

M 334.7

Cryst. (hexane).

Bigorgne, M. *et al*, *J. Organomet. Chem.*, 1970, **24**, 211 (*synth*)
Legendre, J. *et al*, *Bull. Soc. Chim. Fr.*, 1971, 1998 (*cryst struct*)
Bigorgne, M. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 1929 (*ir, raman*)

$C_7H_9FeO_7P$ IC-005728

Tetracarbonyl(trimethyl phosphite-*P*)iron, 9CI

Tetracarbonyl(phosphorous acid)iron trimethyl ester, 8CI

[14878-71-8]

$(MeO)_3PFe(CO)_4$

M 291.9

Bright-yellow cryst. Mp 45-46°. $Subl._{0.01}$ 30°.

Cotton, J.D. *et al*, *Aust. J. Chem.*, 1969, **22**, 2673 (*synth, ir, raman, ms, pmr*)
Udovich, C.A., *Inorg. Chem.*, 1969, **8**, 1066 (*stereochem*)
Mosbo, J.A. *et al*, *J. Magn. Reson.*, 1972, **8**, 243 (*pmr*)
Darensbourg, D.J. *et al*, *Inorg. Chem.*, 1974, **13**, 2135 (*ir*)
Conder, H.L. *et al*, *J. Organomet. Chem.*, 1974, **67**, 93 (*synth*)
Greatrex, R. *et al*, *J. Organomet. Chem.*, 1976, **114**, 199 (*mössbauer*)
Graaf, J.L. *et al*, *Organometallics*, 1982, **1**, 837 (*ir*)

$C_7H_9GeO_4Ru^{\ominus}$ IC-005729

Tetracarbonyl(trimethylgermyl)ruthenate(1 –)

$[Ru(CO)_4(GeMe_3)]^{\ominus}$

M 330.8 (ion)

Only generated in soln., and poorly characterised. Synth. by the reduction of Octacarbonylbis(trimethylgermyl) diruthenium(*I*), IC-008651 with Na/Hg. A useful synthetic reagent. Sol. THF.

Knox, S.A.R. *et al*, *J. Chem. Soc. A*, 1971, 2874 (*synth, reaction*)

$C_7H_9MnO_4P^{\ominus}$ IC-005730

Tetracarbonyl(trimethylphosphine)manganate(1 –), 10CI

$[Mn(PMe_3)(CO)_4]^{\ominus}$

M 243.0 (ion)

K salt: [67236-96-8].

Synth. from $Mn_2(CO)_8(PMe_3)_2$ and $NaK_{2.8}$. Generated and used *in situ*.

King, R.B., *Acc. Chem. Res.*, 1970, **3**, 417 (*synth*)
Ellis, J.E. *et al*, *J. Organomet. Chem.*, 1975, **99**, 263.
Müller, R. *et al*, *J. Organomet. Chem.*, 1978, **150**, C11 (*synth*)

$C_7H_9MnO_7P^{\ominus}$ IC-005731

Tetracarbonyl(trimethyl phosphite-*P*)manganate(1 –), 10CI

[53202-04-3]

$[MnP(OMe)_3(CO)_4]^{\ominus}$

M 291.0 (ion)

Synth. by photolysis of [PPN][$Mn(CO)_5$] and $P(OMe)_3$ in THF.

Bis(triphenylphosphine)iminium salt: [67047-39-6]. Generated in soln. Ir ν_{CO} 1954m, 1858m, 1823vs cm^{-1} (THF).

Faltynek, R.A. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 2701 (*synth, ir*)

$C_7H_9O_4RuSi^{\ominus}$ IC-005732

Tetracarbonyl(trimethylsilyl)ruthenate(1 –)

$[Ru(CO)_4(SiMe_3)]^{\ominus}$

M 286.3 (ion)

Only generated in soln., and poorly characterised. Prepd. by the reduction of Octacarbonylbis(trimethylsilyl) diruthenium, IC-008657 with Na/Hg. A useful synthetic reagent. Sol. THF.

Knox, S.A.R. *et al*, *J. Chem. Soc. A*, 1969, 2559 (*synth, reactions*)

$C_7H_9O_7PRu$ IC-005733

Tetracarbonyl(trimethylphosphite-*P*)ruthenium(0), 10CI

[75641-93-9]

$(OC)_4RuP(OMe)_3$

M 337.1

Trigonal bipyramidal with axial P. Ru—P 230.9 pm. Synth. from $Ru_3(CO)_{12}$, $P(OMe)_3$ and CO (80 atm) in hexane at 125°. White cryst. (turn yellow in sunlight). Mp 41-42°. Ir ν_{CO} 2072, 2002, 1971, 1957 cm^{-1} (hexane).

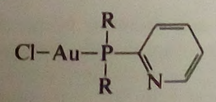
Cobbledick, R.E. *et al*, *J. Organomet. Chem.*, 1980, **195**, 77 (*synth, cryst struct, pmr, cmr, P-31 nmr, ir*)

$C_7H_{10}AuClNP$ IC-005734

Chloro[2-(dimethylphosphino)pyridine-*P*]gold, 11CI

Chloro(dimethyl-2-pyridylphosphine)gold

[83827-03-6]



R = Me

M 371.5

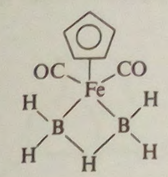
Colourless cryst. (MeOH). Mp 126-127.5°.

Inoguchi, Y. *et al*, *Chem. Ber.*, 1982, **115**, 3085 (*synth*)

$C_7H_{10}B_2FeO_2$ IC-005735

Dicarbonyl(η⁵-2,4-cyclopentadien-1-yl)[η²-pentahydrodiborato(1 –)]iron

[72576-54-6]



M 203.6

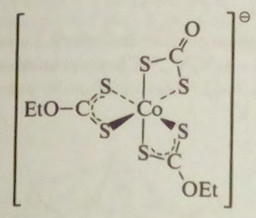
Yellow cryst.; stable at r.t. Sol. CH_2Cl_2. Subl. *in vacuo*.

Plotkin, J.S. *et al*, *J. Organomet. Chem.*, 1979, **182**, C15 (*synth, ir, pmr, ms, B-11 nmr*)

$C_7H_{10}CoO_3S_6^{\ominus}$ IC-005736

(Dithiocarbonato)bis(*O*-ethyldithiocarbonato) cobaltate(*III*)(1 –)

[Carbonodithioato(2 –)-S,S]bis(O-ethylcarbonodithioato-S,S′) cobaltate(III), *10CI. (Dithiocarbonato-S,S′)bis(ethylxanthato) cobaltate*(III)(*1 –*)



M 393.4 (ion)

Approx. octahedral.

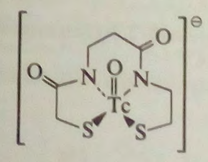
Et_4N salt: Blue cryst.

Raston, C.L. *et al*, *Aust. J. Chem.*, 1978, **31**, 291 (*synth, ir, cryst struct*)

$C_7H_{10}N_2O_3S_2Tc^{\ominus}$ IC-005737

[1,9-Dimercapto-2,6-dioxo-3,7-diazanonanato] oxotechnetate(*V*)(1 –)

[N[N-(*Mercaptoacetyl-β-alanyl*)]*mercaptoethylaminato*] *oxotechnetate*(V)(*1 –*). *Tc-AP-DADS. AP-DADS-Tc*



M 333.2 (ion)

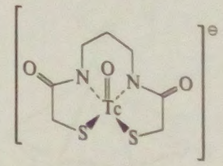
Unsymmetrical isomer of symmetrical Tc-P-DADS. Synth. from $TcO_4^{\ominus}$ and preformed ligand by $SnCl_2$ reduction. Promising renal imaging agent.

Schneider, R.F. *et al*, *J. Nucl. Med.*, 1984, **25**, 223 (*ligand synth*)
McAfee, J.G. *et al*, *J. Nucl. Med.*, 1985, **26**, 375 (*synth, biodistribn*)

$C_7H_{10}N_2O_3S_2Tc^{\ominus}$ IC-005738

Oxo[*N,N′*-1,3-propanediylbis[2-mercaptoacetamidato] (4 –)-*N,N′,S,S′*]technetate(1 –), 10CI

Oxo[N,N′-*propylenebis*(2-*mercaptoacetimido*)]*technetate*(V). *Tc-P-DADS. P-DADS-Tc*



M 333.2 (ion)

This and analogues are representative of complexes of this type. Synth. from $TcO_4^{\ominus}$ + H_4L, with dithionite or $SnCl_2$ reduction. Promising for renal imaging.

Ph_4As salt: [75949-48-3].

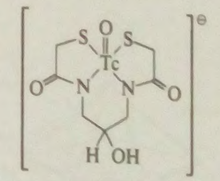
Yellow-orange plates (aq. EtOH). Mp 153-155°.

Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 1629 (*synth, uv, ir, pmr*)
Schneider, R.F. *et al*, *J. Nucl. Med.*, 1984, **25**, 223 (*ligand synth*)
McAfee, J.G. *et al*, *J. Nucl. Med.*, 1985, **26**, 375 (*synth, pharmacol*)

$C_7H_{10}N_2O_4S_2Tc^{\ominus}$ IC-005739

[[*N,N′*-(2-Hydroxy-1,3-propanediyl)bis[2-mercaptoacetamidato]](4 –)-*N,N′,S,S′*]oxotechnetate(*V*) (1 –), 11CI

[103639-39-0]



M 349.2 (ion)

Renal imaging agent - polar groups help renal excretion and specificity.

[103728-99-0]

Kasina, S. *et al*, *J. Med. Chem.*, 1986, **29**, 1933.

$C_7H_{10}NiO_3S$ IC-005740

Tricarbonyl(diethyl sulfide)nickel

Tricarbonyl(ethyl sulfide)nickel

$Ni(CO)_3(SEt_2)$

M 232.9

No phys. props. recorded.

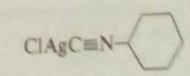
Bouquet, G. *et al*, *Bull. Soc. Chim. Fr.*, 1962, 433 (*synth, ir*)
Benn, R. *et al*, *Organometallics*, 1985, **4**, 209 (*cmr*)

$C_7H_{11}AgClN$ IC-005741

Chloro(isocyanocyclohexane)silver, 9CI

(Cyclohexyl isocyanide)chlorosilver

[55145-55-6]



M 252.4

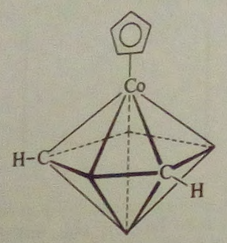
Solid. Insol. common org. solvs. Mp 93-95°.

Minghetti, G. *et al*, *Inorg. Chem.*, 1975, **14**, 1974 (*synth*)

$C_7H_{11}B_4Co$ IC-005742

$(\eta^5$-2,4-Cyclopentadien-1-yl)[(2,3,4,5,6-η)-hexahydro-2,4-dicarbahexaborato(2−)]cobalt, 11CI

[41660-23-5]



M 197.3

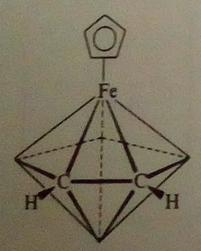
closo-. Air-stable yellow cryst. (heptane). Sol. $CHCl_3$.

Miller, V.R. *et al, J. Am. Chem. Soc.*, 1973, **95**, 2830 (*synth, ir, pmr, B-11 nmr*)
Beer, D.C. *et al, Inorg. Chem.*, 1974, **13**, 1138 (*synth, ir*)
Miller, V.R. *et al, J. Am. Chem. Soc.*, 1975, **97**, 4213 (*pyrol*)
Brennan, D.E. *et al, Inorg. Chem.*, 1982, **21**, 1963 (*props*)

$C_7H_{11}B_4Fe$ IC-005743

$(\eta^5$-2,4-Cyclopentadien-1-yl)[(2,3,4,5,6-η)-hexahydro-2,3-dicarbahexaborato(2−)]iron, 9CI

[38930-35-7]



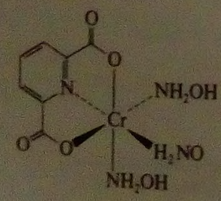
M 194.2

Brown cryst. Paramagnetic.

Sneddon, L.G. *et al, J. Am. Chem. Soc.*, 1972, **94**, 7161; 1973, **95**, 6623 (*synth, ms, pmr, nmr*)

$C_7H_{11}CrN_4O_7$ IC-005744

Hydroxylaminatobis(hydroxylamine)(pyridine-2,6-dicarboxylato)chromium(*III*)



M 315.1

Struct. assumed from $(NO)(H_2O)_2$ analogue. The type of bonding for NH_2OH and H_2NO is not assigned. Dark green cryst. $\mu_{eff} = 3.6\mu_B$ (298K).

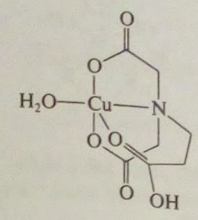
Weighardt, K. *et al, Inorg. Chim. Acta*, 1984, **89**, L43 (*synth*)

$C_7H_{11}CuNO_7$ IC-005745

Aqua[*N*,*N*-bis(carboxymethyl)-β-alaninato(2−)]copper(*II*)

Aqua[[(2-carboxyethyl)imino]diacetato]copper(II). *N,N-Bis(carboxymethyl)-β-alanine, copper complex, 1ZCI*

[109012-65-9]



M 284.7

Contains a six membered chelate ring in boat conform. Dark blue cryst. (hot H_2O). Insol. EtOH, Me_2CO, cold H_2O. H_2O loss starts at 165°. Ir $\nu_{C=O}$ 1718 cm^{-1}.

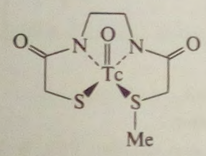
Gonzalez-Garcia, S. *et al, Coord. Chem.*, 1986, **24**, 357 (*synth*)
Nguyen-Huy-Dung, *et al, Inorg. Chem.*, 1987, **26**, 2365 (*synth, cryst struct, ir, props, esr, magnetism*)

$C_7H_{11}N_2O_3S_2Tc$ IC-005746

[*N*-[2-[(Mercaptoacetyl)amino]ethyl]-2-(methylthio)acetamidato(3−)-*N*,*N*′,*S*,*S*′]oxotechnetium(*V*), 12CI

[2-(Methylthio)-N-[2-((thioacetyl)amino)ethyl]-acetamidato]oxotechnetium(V)

[114095-49-7]



M 334.2

Synth. from $Na[TcO(OCH_2CH_2O)_2]$ and ligand in alkaline MeOH. Air-stable deep red needles (CH_2Cl_2/hexane). Sol. polar org. solvs. Mp 191-193°.

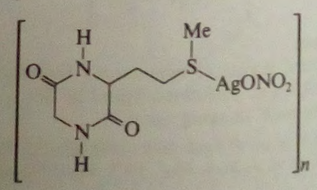
Bryson, N. *et al, Inorg. Chem.*, 1988, **27**, 2154 (*synth, uv, ir, pmr, cmr, ms, conductivity*)

$C_7H_{12}AgN_3O_5S$ IC-005747

[3-[2-(Methylthio)ethyl]-2,5-piperazinedione-*S*](nitrato-*O*,*O*′)silver(*I*), 11CI

(Cyclo-L-methionylglycine)silver(I) *nitrate*

[86339-04-0]



M 358.1

Infinite linear arrays of silver atoms are doubly bridged by sulfur atoms and nitrate groups. Cryst.

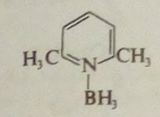
Ettorre, R. *et al, Inorg. Chim. Acta*, 1979, **32**, L39 (*pmr*)
Bressan, M. *et al, Int. J. Pept. Protein Res.*, 1982, **19**, 402 (*synth, ir, nmr*)
Valle, G. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 453 (*cryst struct*)

$C_7H_{12}BN$ IC-005748

(2,6-Dimethylpyridine)trihydroboron, 10CI

(2,6-Dimethylpyridine, compd. with borane (1:1), 9CI. 2,6-Lutidine, compd. with borane (1:1), 8CI. Borane 2,6-dimethylpyridine

[3999-42-6]



M 120.9

Stereoselective reducing agent. White cryst. solid. V. sol. THF, MeOH; insol. hexane. Mp 112-114° (106-107°).

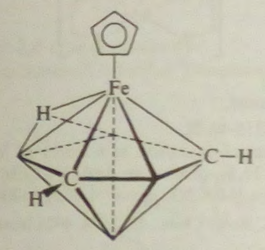
Ryschkewitsch, G.E. *et al, Inorg. Chem.*, 1965, **4**, 575 (*props*)
Brown, H.C. *et al, J. Am. Chem. Soc.*, 1966, **88**, 2520.
Mooney, E.F. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 1439 (*synth, nmr*)
Nöth, H. *et al, Chem. Ber.*, 1974, **107**, 3070 (*nmr*)
Andrews, G.C. *et al, Tetrahedron Lett.*, 1980, **21**, 693, 697 (*use*)

$C_7H_{12}B_4Fe$ IC-005749

$(\eta^5$-2,4-Cyclopentadien-1-yl)[(2,3,4,5,6-η)-heptahydro-2,5-dicarbahexaborato(1−)-H^a]iron, 9CI

π-Cyclopentadienyliron-2,4-$C_2B_4H_6$ hydride

[51177-77-6]



M 195.2

closo-. Red-orange.

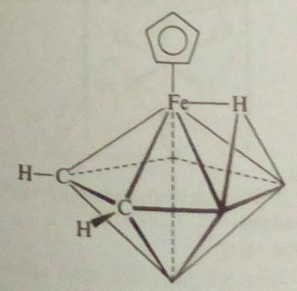
Sneddon, L.G. *et al, J. Am. Chem. Soc.*, 1973, **95**, 6623 (*synth, pmr, ms, nmr, ir*)

$C_7H_{12}B_4Fe$ IC-005750

$(\eta^5$-2,4-Cyclopentadien-1-yl)[(2,3,4,5,6-η)-hexahydro-2,3-dicarbahexaborato(2−)]hydroiron, 9CI

(η^5-2,4-Cyclopentadien-1-yl)[(2,3,4,5,6-η)-heptahydro-4,5-dicarbahexaborato(1−)-H^a]iron, 9CI

[38980-34-6]



M 195.2

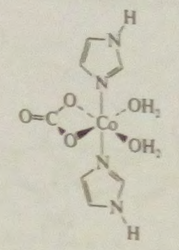
closo-. Diamagnetic orange solid. Sublimes.

Sneddon, L.G. *et al, J. Am. Chem. Soc.*, 1972, **94**, 7161; 1973, **95**, 6623 (*synth, ms, pmr, nmr*)

$C_7H_{12}CoN_4O_5$ IC-005751

Diaquacarbonatobis(imidazole)cobalt(*II*), 8CI

[30579-03-4]



M 291.1

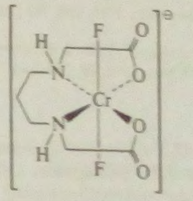
Octahedral with *trans*-imidazole, *cis*-H_2O config. Red-brown cryst. Solid dec. slowly when warmed and rapidly when heated to $[Co(imidazolate)_2]_n$ which is polymeric. Paramagnetic.

Baraniak, E. *et al, J. Chem. Soc. A*, 1970, 2558 (*synth, ir, struct, ms, magnetism*)

$C_7H_{12}CrF_2N_2O_4^{\ominus}$ IC-005752

Difluoro[(1,3-propanediamine)-*N*,*N*′-diacetato-*N*,*N*′,*O*,*O*′]chromate(*III*)

Difluoro[[N,N′-1,3-propanediylbis[glycinato]](2−)-N,N′,O,O′]chromate(III)(*1−*), *11CI*



trans-form

M 278.1 (ion)

The three possible geometric isomers may be separated by chromatog. and distinguished by nmr.

cis-sym-form

Li salt: [102339-59-3].

cis-unsym-form

Li salt: [102339-57-1].

trans-form

Li salt: [102234-93-5].

Red-violet cryst. + $2H_2O$ (aq. MeOH/Me_2CO).

Bianchini, R.J. *et al, Inorg. Chem.*, 1986, **25**, 2129 (*cryst struct, isom, synth, uv-vis, H-2 nmr*)

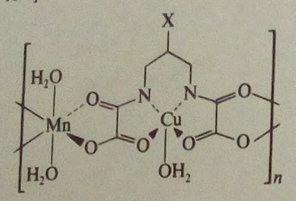
IC-005753

$C_7H_{12}CuMnN_2O_9$

Diaqua(aquacopper)[μ-[[2,2′-(1,3-propanediyl)diiminobis[2-oxoacetato]](4−)]]manganese(*II*), 11CI

catena-*Triaqua*[*μ-1,3-propylene-bis*[*oxamato*]]*copper manganese*(II)

[105121-18-4]



X = H

M 386.6

Polymeric chain struct. with Mn.....Cu 575.1 pm. Synth. from $Mn(ClO_4)_2$ + Na_2[Cu(1,3-propanebis(oxamato))] by slow diffusion of aq. solns. Light blue cryst.; forms a dihydrate. Large intrachain antiferromagnetic interaction, weak interchain antiferromagnetic interaction.

[101935-07-3]

Pei, Y. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 7428 (*synth, cryst struct, magnetism*)

Pei, Y. *et al*, *Inorg. Chem.*, 1987, **26**, 138 (*synth, cryst struct, magnetism*)

Kahn, O. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 782 (*synth, cryst struct, magnetism*)

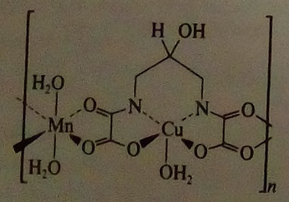
Guillou, O. *et al*, *J. Phys. Colloq. C*, 1988, **8**, 857 (*esr*)

Gatteschi, D. *et al*, *Inorg. Chem.*, 1989, **28**, 287 (*esr*)

$C_7H_{12}CuMnN_2O_{10}$ **IC-005754**

Diaqua(aquacopper)[μ-[2,2′-[(2-hydroxy-1,3-propanediyl)diimino]bis[2-oxoacetato]](4−)]manganese, 11CI

catena-[μ_3-*2-Hydroxy-1,3-propylenebis*[*oxamato*]]*aquacopper*(II)*diaquamanganese*(II)



M 402.6

Ordered bimetallic chain struct. Synth. from $Mn(ClO_4)_2.6H_2O$ and Na_2[CuL]. Blue single cryst. Orders ferromagnetically at 4.6K.

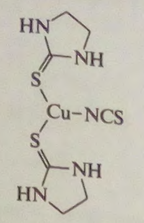
Pei, Y. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 782 (*synth, cryst struct, magnetism*)

Gatteschi, D. *et al*, *Inorg. Chem.*, 1989, **28**, 287 (*esr*)

$C_7H_{12}CuN_5S_3$ **IC-005755**

Bis(imidazolidine-2-thione)(thiocyanato-*N*)copper(*I*)

[119676-61-8]



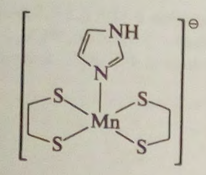
M 325.9

Colourless cryst. (EtOH/MeCN).

Raper, E.S. *et al*, *Inorg. Chim. Acta*, 1989, **155**, 85 (*synth, cryst struct, ir*)

$C_7H_{12}MnN_2S_4^{\ominus}$ **IC-005756**

Bis[1,2-ethanedithiolato(2−)-*S,S′*](1*H*-imidazole-*N*^{3})manganate(*III*)(1−), 11CI



M 307.3 (ion)

Square pyramidal.

Et_4N salt: [96316-46-0].

Synth. by aerial oxidation of a slurry of $MnCl_2.4H_2O$, $Na_2[SCH_2CH_2S]$, imidazole, and $[NEt_4]Br$ in EtOH. Black prisms (MeCN). μ_{eff} = 4.97μ_B (300K).

Seela, J.L. *et al*, *Inorg. Chem.*, 1985, **24**, 4455 (*synth, cryst struct, magnetism*)

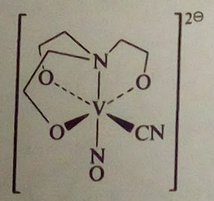
Seela, J.L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 58 (*synth, cryst struct, electrochem*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 46 (*rev, bibl*)

$C_7H_{12}N_3O_4V^{2\ominus}$ **IC-005757**

Cyano(2,2′,2″-nitrilotriethoxy)nitrosylvanadate(*I*)(2−)

(*Cyano*-C)[[*2,2′,2″-nitrilotris*[*ethanolato*]](3−)-N,O,O′,O″]*nitrosylvanadate*(2−), *11CI. Cyano*[*triethanolaminato*(3−)]*nitrosylvanadate*(I)(2−)



M 253.1 (ion)

See also [[2,2′,2″-Nitrilotris[ethanolato]](3−)-*N,O,O′,O″*]nitrosylvanadate(1−), IC-005150.

Ba salt: [101754-18-1].

Synth. by reaction of NH_4VO_3, triethanolamine, hydroxyammonium chloride and NaOH in H_2O, then adding NaCN and $BaCl_2$. Blue solid + $5H_2O$ (H_2O). Ir ν_{CN} 2100 cm^{-1}, ν_{NO} 1450 cm^{-1}. Interatomic distance; N—O 125.1 pm.

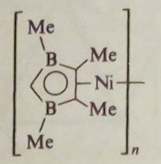
Wieghardt, K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 2493 (*synth, cryst struct, ir, uv-vis*)

$C_7H_{13}B_2Ni$ **IC-005758**

(1,3,4,5-Tetramethyl-1,3-diborolyl)nickel

(*2,4,5-η*)-*2,3-Dihydro-1,3,4,5-tetramethyl-1*H-*1,3-diborol-2-yl-*B^1,B^3]*nickel*

[99884-61-4]



M 177.4

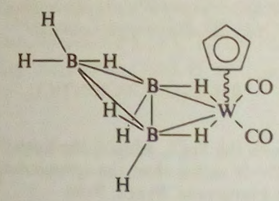
Polymeric "polydecker sandwich" compd. Black air-sensitive cryst. Insol. org. solvs. Stable to 500°.

Kuhlmann, T. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1986, **25**, 105 (*synth*)

$C_7H_{13}B_3O_2W$ **IC-005759**

Dicarbonyl(η^5-2,4-cyclopentadien-1-yl)[octahydrotriborato(1−)-*H*^{1},*H*^{3}]tungsten, 10CI

[65452-39-3]



M 345.4

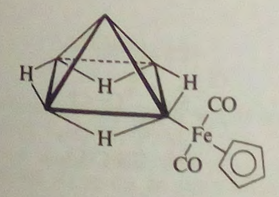
arachno-. Air-stable orange/brown oil (by chromatog., THF). Sol. CH_2Cl_2, $CHCl_3$, THF, Me_2CO.

Gaines, D.F. *et al*, *Inorg. Chem.*, 1978, **17**, 794 (*synth, B-11 nmr, pmr, deriv*)

$C_7H_{13}B_5FeO_2$ **IC-005760**

Dicarbonyl(η^5-2,4-cyclopentadien-1-yl)[(2-η)-octahydropentaborato(1−)]iron, 10CI

[67087-72-3]



M 239.0

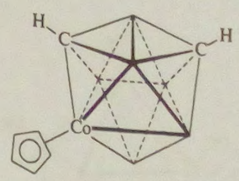
Air-stable orange solid. Sol. most org. solvs.

Greenwood, N.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 237 (*synth, ir, ms, pmr, B-11 nmr*)

$C_7H_{13}B_6Co$ **IC-005761**

(η^5-2,4-Cyclopentadien-1-yl)[(3,5,6,7,8-η)-octahydro-4,5-dicarbaoctaborato(2−)]cobalt, 9CI

[42802-13-1]



M 220.9

Proposed struct. shown. Dark red cryst. solid (by subl.). Sol. CH_2Cl_2, $CHCl_3$, MeCN. Mp 61-64°. Rearranges to 2,6-dicarba isomer on heating.

Dunks, G.B. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 7213 (*synth*)

Evans, W.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 4565 (*synth, uv, ir, B-11 nmr*)

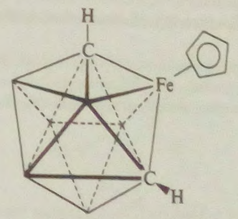
Weiss, R. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 1036 (*pmr, B-11 nmr*)

$C_7H_{13}B_6Fe$ **IC-005762**

(η^5-2,4-Cyclopentadien-1-yl)[(1,3,6,8-η)-octahydro-1,8-dicarbaoctaborato(2−)]iron, 9CI

4-(*η-Cyclopentadienyl*)-*4,1,8-FeC$_2$B$_6$H$_8$*

[42808-85-5]



M 217.8

Red cryst. (hexane). Mp 132-133°. Paramagnetic. Reduced to a diamagnetic purple Fe(*II*) deriv.

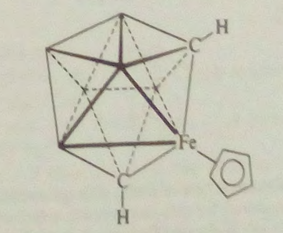
Evans, W.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 4565 (*synth, ms, uv, ir, polarog, pmr, nmr*)

$C_7H_{13}B_6Fe$ **IC-005763**

(η^5-2,4-Cyclopentadien-1-yl)[(3,5,6,7,8-η)-octahydro-5,6-dicarbaoctaborato(2−)]iron, 9CI

1-(*η^5-Cyclopentadienyl*)-*1,4,6-FeC$_2$B$_6$H$_8$*. *4,6-π-Cyclopentadienyliron-C$_2$B$_6$H$_8$*

[42968-39-8]



M 217.8

Brown cryst. (hexane). Paramagnetic. Reduced to a diamagnetic Fe(*II*) species.

Evans, W.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 4565 (*synth, ms, uv, ir, polarog, pmr, nmr*)

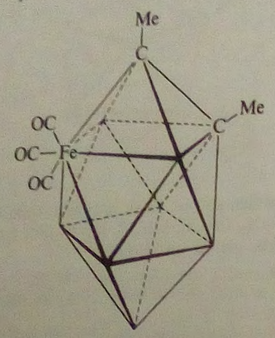
IC-005764

$C_7H_{13}B_7FeO_3$

Tricarbonyl[η⁵-heptahydro-*C,C'*-dimethyldicarbanonaborato(2−)]iron, 10CI

2,1,4-(Tricarbonyliron)-1,4-dimethyl-$C_2B_7H_7$

[64103-53-3]



M 276.7

closo-. Air-stable, light-sensitive bright-yellow cryst.(hexane). $Bp_{0.0001}$ 25° subl.

Maxwell, W.M. *et al*, *Inorg. Chem.*, 1977, **16**, 3094 (*synth, ir, ms, nmr, pmr*)

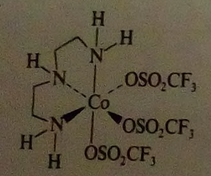
IC-005765

$C_7H_{13}CoF_9N_3O_9S_3$

Diethylenetriaminetris(trifluoromethanesulfonato)cobalt(*III*)

Tris(trifluoromethanesulfonato)[N-(2-aminoethyl)-1,2-ethanediamine]cobalt. [N-(2-Aminoethyl)-1,2-ethanediamine-N,N',N'']*tris(trifluoromethanesulfonato*-O)*cobalt, 10CI*

[75522-53-1]



M 609.3

fac-form only known. Purple solid. Sol. F_3CSO_3H, H_2O.

Inorg. Synth., 1983, **22**, 104 (*synth, uv, props*)

Dixon, N.E. *et al*, *Inorg. Chem.*, 1981, **20**, 470 (*synth, uv, kinetics*)

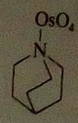
IC-005766

$C_7H_{13}NO_4Os$

(1-Azabicyclo[2.2.2]octane)tetraoxoosmium(*VIII*), 10CI

Tetraoxoquinuclidineosmium(VIII)

[63891-08-7]



M 365.3

Synth. by direct reaction of OsO_4 with quinuclidine. Starting material for oxo-osmium(*VI*) esters which may be hydrol. to *cis*-glycols. Red platelets (CCl_4). Mp 130-132°.

Cleare, M.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 941 (*synth, ir, uv*)

Griffith, W.P. *et al*, *Inorg. Chim. Acta*, 1978, **31**, L413 (*cryst struct*)

Schroder, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1607 (*use*)

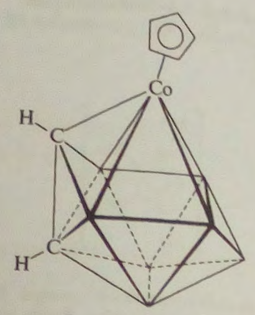
IC-005767

$C_7H_{14}B_7Co$

(η⁵-2,4-Cyclopentadien-1-yl)[(4,5,6,8,9-η)-nonahydro-1,4-dicarbanonaborato(2−)]cobalt

2-(η-Cyclopentadienyl)cobalta-1,4-dicarbadecaborane(9)

[99531-65-4]



M 232.7

Red solid (by chromatog. C_6H_6/hexane). Sol. C_6H_6. Isomerises at 50° in 12 hrs.

Briguglio, J.J. *et al*, *Organometallics*, 1986, **5**, 327 (*synth, pmr, B-11 nmr, ir, ms*)

IC-005768

$C_7H_{14}Cl_4N_2Ti$

Tetrachloro(diisopropylcyanamide)titanium(*IV*)

[*Bis(1-methylethyl)cyanamide*]*tetrachlorotitanium*(IV), *11CI*

Titanium(IV) *chloride diisopropylcyanamide*

[89953-11-7]

$$[(H_3C)_2CH]_2NC{\equiv}NTiCl_4$$

M 315.8

By analogy with the $SbCl_5$ adduct, the ligand appears to be $R_2N{-}C{-}N$ rather than the symmetrically substituted cyanamide. Synth. from diisopropylcyanamide + $TiCl_4$ in CH_2Cl_2. Yellow hygroscopic solid. Mp 72-73°.

Jochims, J.C. *et al*, *Chem. Ber.*, 1984, **117**, 1161 (*synth, ir, pmr, cmr*)

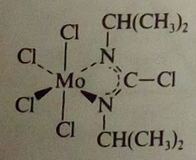
IC-005769

$C_7H_{14}Cl_5MoN_2$

Tetrachloro(*N,N'*-diisopropylchlorocarbodiimidato-*N,N'*)molybdenum(*V*)

[N,N'-*Bis(1-methylethyl)carbamimidic chloridato*-N,N'] *tetrachloromolybdenum*(V), *11CI*

[97311-99-4]



M 399.4

Octahedral. Synth. from $MoCl_5$ + diisopropylcarbodiimide. Dark green cryst. Mp 101° dec. Ir ν_{Mo-N} 516 cm^{-1}.

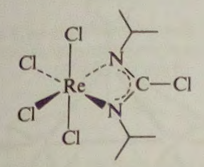
Rajca, G. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **522**, 83 (*cryst struct, synth, ir*)

IC-005770

$C_7H_{14}Cl_5N_2Re$

[*N,N'*-Bis(1-methylethyl)carbamimidic chloridato-*N,N'*]tetrachlororhenium(*V*), 11CI

[97312-00-0]



M 489.6

Octahedral. Synth. from $ReCl_5$ and diisopropyl carbodiimide in CH_2Cl_2 suspension. Dark red brown cryst. Mp 99°.

Rajca, G. *et al*, *Z. Anorg. Allg. Chem.*, 1985, **522**, 83 (*synth, ir*)

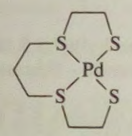
IC-005771

$C_7H_{14}PdS_4$

[[2,2'-[1,3-Propanediylbis(thio)]bis[ethanethiolato]](2−)-*S,S',S'',S'''*]palladium, 10CI

(1,9-Dithiolato-3,7-dithianonane)palladium(II)

[72137-93-0]



M 332.8

Yellow solid. Sol. $CHCl_3$, CH_2Cl_2. Mp 200-205° dec. Contrast formn. of Ni(*II*) trimer Bis(3,7-dithianonane-1,9-dithiolato)trinickel(*II*)(2+), IC-008752.

Roundhill, D.M., *Inorg. Chem.*, 1980, **15**, 557 (*synth, ir*)

IC-005772

$C_7H_{15}AuNP$

Cyano(triethylphosphine)gold

[90981-41-2]

$$Et_3PAuCN$$

M 341.1

Fine white cryst. Sol. toluene, $CHCl_3$. Mp 112.7-113.1°. Disproportionates in soln. to $(Et_3P)_2Au^{\oplus}$ and $Au(CN)_2^{\ominus}$. Ir $\nu_{C{\equiv}N}$ 2138 cm^{-1} (solid).

Hormann, A.L. *et al*, *Inorg. Chem.*, 1986, **25**, 3953 (*synth, cryst struct, mössbauer, nmr, cmr*)

IC-005773

$C_7H_{15}AuNPS$

(Thiocyanato-*S*)(triethylphosphine)gold, 9CI

[14243-46-0]

$$Et_3PAuSCN$$

M 373.2

Shows antiarthritic activity. Cryst. (EtOH aq.). Sol. $CHCl_3$, EtOH, C_6H_6. Mp 50-51°.

Coates, G.E. *et al*, *Aust. J. Chem.*, 1966, **19**, 539 (*synth*)

Ger. Pat., 2 434 920, (1975); *CA*, **83**, 84857j (*synth, use*)

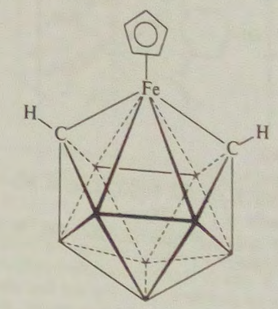
IC-005774

$C_7H_{15}B_8Fe$

(η⁵-2,4-Cyclopentadien-1-yl)[(5,6,7,8,9,10-η)-decahydro-6,9-dicarbadecaborato(2−)]iron, 10CI

1,2,3-π-Cyclopentadienyliron-$C_2B_8H_{10}$

[42769-15-3]



M 241.5

Red-brown needles (CH_2Cl_2/hexane). Mp 275-277°. Paramagnetic. May be reduced to diamagnetic species.

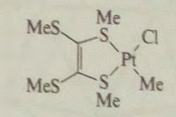
Evans, W.J. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 4565 (*synth, uv, ir, ms, electrochem*)

IC-005775

$C_7H_{15}ClPtS_4$

Chloro(methyl)[1,1,2,2-tetrakis(methylthio)ethene]platinum(*II*), 11CI

[86567-87-5]



M 457.9

Probably square planar struct. Pale yellow needles ($CHCl_3$/pet. ether). Sol. CH_2Cl_2/CS_2 (1:1). Mp 158-159°.

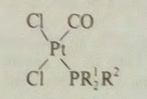
Abel, E.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 1017 (*synth, pmr*)

IC-005776

$C_7H_{15}Cl_2OPPt$

Carbonyldichloro(triethylphosphine)platinum, 10CI

Dichlorocarbonyl(triethylphosphine)platinum



cis-form

$R^1 = R^2 = Et$

M 412.1

cis-form [65466-58-2]

Cryst. (EtOH). Mp 134-136°. Dipole moment 10.0 D.

trans-form [73347-27-0]

Obt. in soln. only. Readily isom. to *cis*-form, isom. catalysed by CO.

Chatt, J. *et al*, *J. Chem. Soc.*, 1964, 1662 (*synth, ir*)

Manojlović-Muir, L. *et al*, *J. Organomet. Chem.*, 1977, **142**, 265 (*struct*)

Anderson, G.K. *et al*, *J. Chem. Res. (S)*, 1979, **5**, 120 (*nmr*)

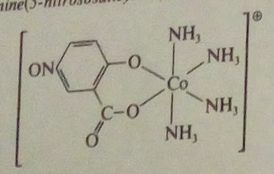
Anderson, G.K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1988 (*synth, ir, nmr*)

IC-005777

$C_7H_{15}CoN_5O_4^{\oplus}$

Tetraammine[2-hydroxy-5-nitrosobenzoato(2−)-O^1,O^2]cobalt(*III*)(1+), 1Cl

Tetraammine(5-nitrososalicylato)cobalt(III)(*1+*)



M 292.1 (ion)

Chloride: [81489-32-9].
Brown solid (H_2O). Sol. H_2SO_4. Dec. at 160-163°.
Paramagnetic; $\mu_{eff} = 2.84\mu_B$.

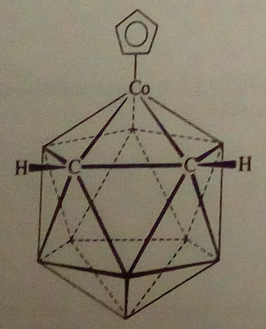
Yamamoto, Y. *et al, Bull. Chem. Soc. Jpn.*, 1982, **55**, 136 (*synth, ir, uv, magnetism*)

IC-005778

$C_7H_{16}B_9Co$

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]cobalt, 11Cl

[37100-20-2]



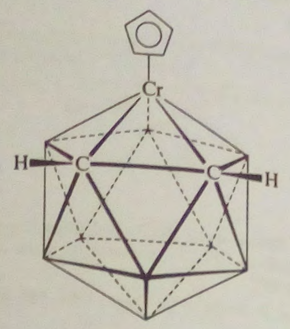
M 256.4

closo-. Air-stable yellow cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2, Me_2CO, MeCN. Mp 246°. Dicarbollyl ligand undergoes rearrangement upon heating vapour to 400-500°.

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, ir, uv, pmr*)
Kaloustian, M.K. *et al, J. Am. Chem. Soc.*, 1972, **94**, 6679 (*synth, ir, uv, pmr, props*)
Jones, C.J. *et al, Inorg. Chem.*, 1973, **12**, 608 (*synth*)
Stibr, B. *et al, Inorg. Chem.*, 1983, **22**, 237 (*synth*)
Gennett, T. *et al, J. Electroanal. Chem. Interfacial Electrochem.*, 1985, **186**, 179 (*props*)
Smith, D.E. *et al, Organometallics*, 1986, **5**, 760 (*cryst struct*)

$C_7H_{16}B_9Cr$ IC-005779

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]chromium



M 249.4

Presumed *closo-* struct. Dark red cryst. (C_6H_6/hexane). Sol. C_6H_6, MeCN. Mp 248-249°. Thermally stable up to Mp.

Ruhle, H.W. *et al, Inorg. Chem.*, 1968, **7**, 2279 (*synth, ir, uv-vis*)

$C_7H_{16}B_9Cr$ IC-005780

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydro-7,9-dicarbaundecaborato(2−)]chromium

M 249.4

Dark red cryst. (C_6H_6/hexane). Sol. C_6H_6. Mp 217-218°. Thermally stable to Mp.

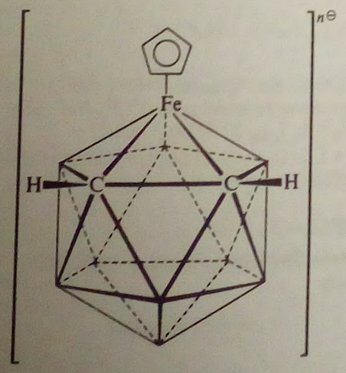
Ruhle, H.W. *et al, Inorg. Chem.*, 1968, **7**, 2279 (*synth, ir, uv-vis*)

$C_7H_{16}B_9Fe^{\ominus}$ IC-005781

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]ferrate(1−), 9Cl

[Undecahydrodicarbaundecaborato(2−)] cyclopentadienylferrate(2−)

[37185-23-2]



n = 1

M 253.3 (ion)

closo-. Diamagnetic.

Me_4N salt: Orange plates (EtOH). Mp 158°.

Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, pmr, uv, ir*)

IC-005782

$C_7H_{16}B_9Fe$

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]iron, 9Cl

π-Cyclopentadienyliron-π-(3)-1,2-$B_9C_2H_{11}$

[11070-70-5]

As (η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]ferrate(1−), IC-005781 with

n = O

M 253.3

Mediator in an analytical method which provides a direct assay for H_2O_2 down to $<10^{-6}M$. Purple needles (C_6H_6/cyclohexane). Sol. MeCN, Me_2CO. Mp 181-182°. Paramagnetic.

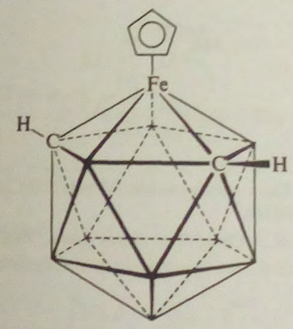
Zalkin, A. *et al, J. Am. Chem. Soc.*, 1965, **87**, 3988 (*cryst struct*)
Hawthorne, M.F. *et al, J. Am. Chem. Soc.*, 1968, **90**, 879 (*synth, ir, uv, polarog, nmr*)
Herber, R.H., *Inorg. Chem.*, 1969, **8**, 174 (*mössbauer*)
Wiersema, R.J. *et al, J. Am. Chem. Soc.*, 1974, **96**, 761 (*cmr, nmr*)
Ammeter, J.H., *J. Magn. Reson.*, 1978, **30**, 299 (*esr*)
U.K. Pat., 33 917, (1983); *CA*, **104**, 3119x (*electrochem*)
Zakharkin, L.I. *et al, Zh. Obshch. Khim.*, 1983, **53**, 2153 (*deriv*)
Vasyukova, N.I., *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1984, **10**, 2246 (*ms*)
Frew, J.E. *et al, J. Electroanal. Chem. Interfacial Electrochem.*, 1986, **201**, 1 (*props*)

$C_7H_{16}B_9Fe$ IC-005783

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-undecahydro-7,9-dicarbaundecaborato(2−)]iron

π-Cyclopentadienyl-(π-7,9-$B_9C_2H_{11}$)iron

[40958-61-0]



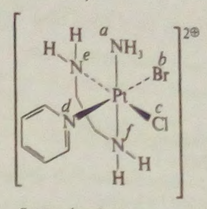
M 253.3

Green. Paramagnetic. Can be reduced to diamagnetic Fe(*II*) species.

Dustin, D.F. *et al, J. Am. Chem. Soc.*, 1973, **95**, 1109 (*synth, pmr, ir, nmr*)
Wiersema, R.J. *et al, J. Am. Chem. Soc.*, 1974, **96**, 761 (*esr*)

$C_7H_{16}BrClN_4Pt^{2\oplus}$ IC-005784

Amminebromochloro(ethylenediamine) pyridineplatinum(*IV*)



a-ammine-b-bromo-c-chloro-e,f-ethylenediamine-d-pyridine-form

M 466.6 (ion)

Three isomers and some enantiomers prepared by use of *trans*-effect. No common standard nomenclature for isomers. Discrimination between structs. is based on synthesis, and has not been confirmed by structural methods. Assignment of registry numbers is tentative.

a-Ammine-b-bromo-c-chloro-e,f-ethylenediamine-d-pyridine-form

Dichloride: [30904-76-8].
Light yellow solid. Sol. EtOH.

a-Ammine-b-bromo-d-chloro-c,f-ethylenediamine-e-pyridine-form

Dichloride: [17112-09-3].
Bright red solid.
Nitrate: [29663-17-0].

a-Ammine-f-bromo-b-chloro-c,d-ethylenediamine-e-pyridine-form

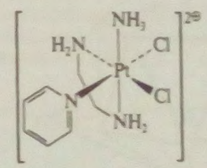
Dichloride: [30904-74-6].
Light green solid.

Chernyaev, I.I. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1966, **11**, 924, 1348 (*synth, uv-vis, ord*)

$C_7H_{16}Cl_2N_4Pt^{2\oplus}$ IC-005785

Amminedichloro(ethylenediamine)pyridineplatinum(*IV*) (2+), 8Cl

Amminedichloro(1,2-ethanediamine-N,N')(pyridine) platinum(2+), 10Cl



a-ammine-b,c-dichloro-d-pyridine-form

M 422.2 (ion)

Distinction between isomers is based on chiroptical spectra and syntheses using *trans* effect rather than crystallography.

(±)-*a-ammine-b,c-dichloro-d-pyridine-form*

Has been resolved.

Dichloride: [17099-27-3].
White cryst.

(±)-*a-ammine-b,f-dichloro-e-pyridine-form*

Dichloride: Solid. Dec. on heating to 100° with loss of Py.

(±)-*a-ammine-b,d-dichloro-c-pyridine-form*

Chloride, nitrate: [73035-94-6].
Cryst.

[17112-65-1, 17112-66-2, 17992-30-2, 18324-09-9, 30904-73-5, 30904-75-7]

Chernyaev, I.I. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1966, **11**, 719, 723 (*resoln*)
Fedotova, T.N. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 1272.
Fedotova, T.N. *et al*, *Koord. Khim.*, 1976, **2**, 1260.

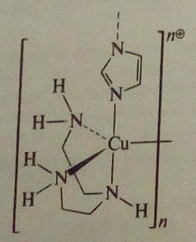
IC-005786

$C_7H_{16}CuN_5^{\oplus}$

***catena*-(Diethylenetriamine-*N,N′,N″*)imidazolatocopper(*II*)(1+)**

[N-(*2-Aminoethyl*)-*1,2-ethanediamine*-N,N′,N″](*1H-imidazolato*-N′)*copper*(II)(*1+*), *11Cl*

[95780-75-9]



M 233.7 (ion)

Polymeric with imidazole bridges and trigonal bipyramidal copper.

Perchlorate: [105204-10-2].
Pale blue fine cryst. Insol. EtOH.
▷ Potentially explosive.

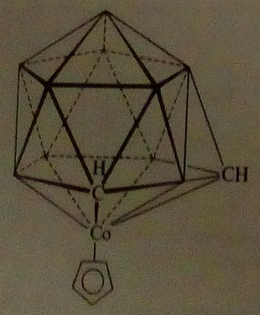
Sato, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1949 (*synth, cryst struct, uv, props*)
Sato, M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1987, 839 (*reactions*)

IC-005787

$C_7H_{17}B_{10}Co$

(η⁵-2,4-Cyclopentadien-1-yl)[η⁶-dodecahydro-1,3-dicarbadodecaborato(2−)]cobalt

[41077-33-2]



red-form

M 268.2

Red cryst. Sol. Me_2CO, MeCN. Mp 250-251°. 2 other isomers known as red-orange, and orange forms also reported.

[52649-54-4, 52649-55-5, 53445-22-0, 53596-04-6]

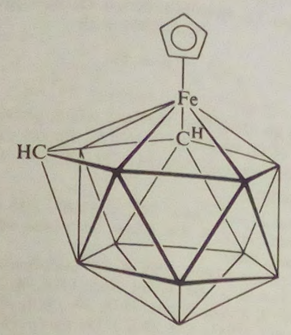
Hawthorne, M.F. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 2541 (*pmr, B-11 nmr, uv-vis*)
Dustin, D. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 1109 (*synth, pmr, B-11 nmr, ir, uv-vis*)
Churchill, M.R. *et al*, *Inorg. Chem.*, 1974, **13**, 1411 (*cryst struct*)

$C_7H_{17}B_{10}Fe$ IC-005788

(η⁵-2,4-Cyclopentadien-1-yl)[η⁶-dodecahydrodicarbadodecaborato(2−)]iron, 9CI

(*η⁵-2,4-Cyclopentadien-1-yl*)[(*7,8,9,10,11,12-η*)-*dodecahydro-7,9-dicarbadodecaborato*(2−)]*iron*

[41077-34-3]



M 265.1

Paramagnetic. Violet. $\mu_{eff} = 2.12\mu_B$. Easily reduced to an orange diamagnetic anionic Fe(*II*) species.

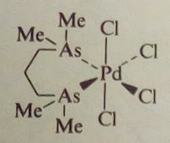
Dustin, D.F. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 1109 (*synth, polarog, pmr, nmr, uv, ir*)

$C_7H_{18}As_2Cl_4Pd$ IC-005789

Tetrachloro[1,3-propanediylbis[dimethylarsine]-*As,As′*]palladium(*IV*)

[*1,3-Bis*(*dimethylarsino*)*propane*]*tetrachloropalladium*(IV)

[85744-76-9]



M 500.2

Octahedral. Dark orange solid. Sl. sol. CH_2Cl_2, MeCN; dec. by DMSO.

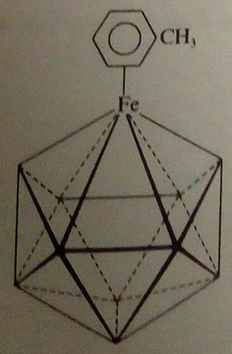
Gray, L.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 133 (*synth, ir, uv-vis*)

$C_7H_{18}B_{10}Fe$ IC-005790

[η⁶-Decahydrodecaborato(2−)][(1,2,3,4,5,6-η)-methylbenzene]iron, 11Cl

1-(*η⁶-Toluene*)-*1-ferraundecaborane*

[92543-05-0]



M 266.1

closo-struct. postulated. Air-sensitive yellow solid (by chromatog. C_6H_6/hexane). Sol. C_6H_6, CH_2Cl_2.

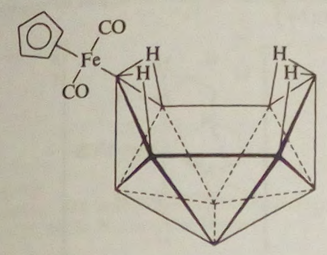
Sneddon, L.G. *et al*, *Inorg. Chem.*, 1984, **23**, 3992 (*synth, B-11 nmr*)

IC-005791

$C_7H_{18}B_{10}FeO_2$

Dicarbonyl(η⁵-2,4-cyclopentadien-1-yl)(decaboran(14)-6-yl)iron, 10CI

[57395-40-1]



M 298.1

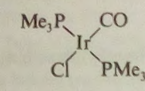
Sol. CH_2Cl_2. Mp 153° dec.

Sato, F. *et al*, *J. Organomet. Chem.*, 1975, **86**, 243 (*synth, ir, pmr, B-11 nmr*)

$C_7H_{18}ClIrOP_2$ IC-005792

Carbonylchlorobis(trimethylphosphine)iridium, 9CI

Carbonylbis(*trimethylphosphine*)*iridium chloride*



M 407.8

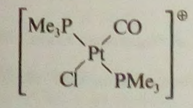
trans-form [21209-86-9]

Air-sensitive yellow prisms (MeOH). Mp >140° dec. $Subl._{0.1}$130°. Ir ν_{CO} 1938 cm^{-1} (nujol).

Deeming, A.J. *et al*, *J. Chem. Soc. A*, 1968, 1887 (*synth, ir, pmr*)
Inorg. Synth., 1978, **18**, 62 (*synth, ir, pmr*)

$C_7H_{18}ClOP_2Pt^{\oplus}$ IC-005793

Carbonylchlorobis(trimethylphosphine)platinum(1+)



M 410.6 (ion)

trans-form

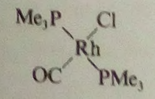
Hexafluorophosphate: [115941-43-0].
$C_7H_{18}ClF_6OP_3Pt$ M 555.6
Cryst. (CH_2Cl_2/Et_2O). Ir ν_{CO} 2115 cm^{-1}(nujol).

Ramprasad, D. *et al*, *Inorg. Chem.*, 1988, **27**, 3151 (*synth, ir, pmr, P-31 nmr, props*)

$C_7H_{18}ClOP_2Rh$ IC-005794

Carbonylchlorobis(trimethylphosphine)rhodium

[36713-95-8]



M 318.5

▷ Catalyst in synth. of phenylsilanes.

trans-form

Pale-yellow cryst. (pet. ether). Sol. CH_2Cl_2, $MeNO_2$. Mp 108° dec. Ir ν_{CO} 1965 cm^{-1} (hexane).

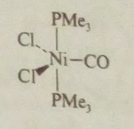
[22710-50-5]

Browning, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, ir, nmr*)
Vastag, S. *et al*, *J. Mol. Catal.*, 1979, **5**, 189 (*ir*)
U.S. Pat., 44 74 976, (1983); *CA*, **101**, 230769 (*use*)

$C_7H_{18}Cl_2NiOP_2$ IC-005795

Carbonyldichlorobis(trimethylphosphine)nickel, 11CI

[70252-75-4]



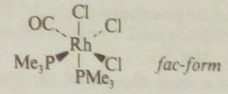
M 309.7

Dark-brown cryst. (Me_2CO). Ir ν_{CO} 2005 cm^{-1}.

Elbaze, G. *et al*, *Inorg. Chim. Acta*, 1984, **85**, L3 (*synth, ir, P-31 nmr, cryst struct*)

$C_7H_{18}Cl_3OP_2Rh$ IC-005796

Carbonyltrichlorobis(trimethylphosphine)rhodium



fac-form

M 389.4

Fac-form

cis-*form*

Formed when Carbonylchlorobis(trimethylphosphine)rhodium, IC-005794 is chlorinated in CH_2Cl_2. Yellow cryst. Sl. sol. CH_2Cl_2, insol. Et_2O. Mp 130° dec. Ir ν_{CO} 2094 cm^{-1} (nujol).

Mer-form

trans-*form*

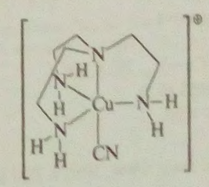
Formed in soln. when Carbonylchlorobis(trimethylphosphine)rhodium, IC-005794 is chlorinated in C_6H_6. Partly isomerises to *fac*-form when isolation is attempted. Ir ν_{CO} 2077 cm^{-1} (C_6H_6).

Browning, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2061 (*synth, nmr, ir*)

$C_7H_{18}CuN_5^{\oplus}$ IC-005797

[*N,N*-Bis(2-aminoethyl)-1,2-ethanediamine-*N,N′,N″,N‴*](cyano-*C*)copper(1+), 9CI

Cyano(*2,2′,2″-triaminotriethylamine*)*copper*(II)(*1+*), *Cyano*[*tris*(*2-aminoethyl*)*amine*]*copper*(II)



M 235.7 (ion)

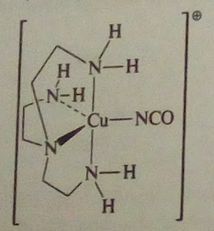
Monomeric units are loosely associated into dimers via H-bonds between NH and NC (Cu—Cu distance 609 pm). Similar complexes prepd. with Cl or Br replacing CN.

Tetraphenylborate: [51464-43-8].
Blue cryst. (MeCN). Sol. MeCN.

Duggan, D.M. *et al, ACS Symp. Ser.*, 1974, **5**, 76 (*magnetism*)
Duggan, D.M. *et al, Inorg. Chem.*, 1974, **13**, 1911, 2929 (*synth, cryst struct, derivs, ir, magnetism, esr*)
Laskowski, E.J. *et al, Inorg. Chem.*, 1975, **14**, 2449 (*derivs, cryst struct*)

$C_7H_{18}CuN_5O^{\oplus}$ IC-005798

(Cyanato-*N*)[tris(2-aminoethyl)amine]copper(*II*)(1+)



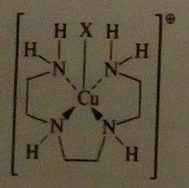
M 251.7 (ion)
Distorted trigonal bipyramidal Cu environment. Described as outer-sphere dimer, with hydrogen bonds linking $[Cu(tren)NCO]^{\oplus}$ units. Exists in two cryst. forms.

Dimer, bis(tetraphenylborate): [52699-44-2]. *Bis*[N,N-*bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*bis*[*μ*-(*cyanato*-N:O)]*dicopper*(2+) *bis*(*tetraphenylborate*), *9CI*
Blue needles (MeCN).

Duggan, D.M. *et al, Inorg. Chem.*, 1974, **13**, 2929 (*synth, magnetism, esr, ir*)
Laskowski, E.J. *et al, Inorg. Chem.*, 1975, **14**, 2449 (*cryst struct*)

$C_7H_{18}CuN_5S^{\oplus}$ IC-005799

(Thiocyanato)(triethylenetetramine)copper(*II*)(1+)
[N,N′-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]
(*thiocyanato*)*copper*(II)(*1+*), *11CI*



X = —NCS

M 267.8 (ion)
Square pyramidal at Cu.

N-bonded-form

Perchlorate: [32371-12-3].
Cryst. (MeOH).
▷ Potentially explosive.

S-bonded-form

Cu—S 260.7, Cu—N_{ax} 201.6 pm.

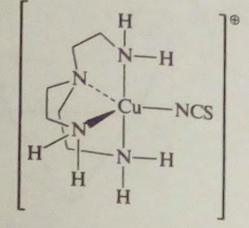
Thiocyanate: [24555-89-3].
Blue prismatic cryst.

[53861-23-7]

Marongiu, G. *et al, Inorg. Chem.*, 1969, **8**, 2763 (*cryst struct, S-bonded*)
Barbucci, R. *et al, J. Chem. Soc. A*, 1969, 1775 (*S-bonded, synth*)
Hathaway, B.J. *et al, J. Chem. Soc. A*, 1971, 1442 (*esr, uv-vis*)
Paoletti, P. *et al, J. Chem. Soc. A*, 1971, 1637 (*ir, uv-vis, synth, both forms*)
Ponticelli, G. *et al, Indian J. Phys., A*, 1982, **56**, 358 (*N-bonded, esr*)
Chary, M.N. *et al, Indian J. Pure Appl. Phys.*, 1984, **22**, 188 (*N-bonded, esr*)
Reddy, K.V.G. *et al, Indian J. Phys., A*, 1985, **59**, 73 (*pmr*)

$C_7H_{18}CuN_5S^{\oplus}$ IC-005800

[Tris(2-aminoethyl)amine](thiocyanato-*N*)copper(*II*)(1+)
β,β′,β″-Triaminotriethylamine(*isothiocyanato*)*copper*(II)(*1+*)
[*4*-(*2-Aminoethyl*)*diethylenetriamine*](*isothiocyanato*)*copper*(II)(*1+*)



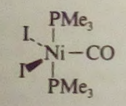
M 267.8 (ion)
Trigonal bipyramidal cation.

Thiocyanate: [15338-54-2].
Dark blue cryst. Mp 187° dec. Ir ν_{CN} 2094s, 2060s; ν_{CS} 818m, 745m cm^{-1}.

Raymond, K.N. *et al, Inorg. Chem.*, 1966, **5**, 1632 (*synth, ir, electrochem*)
Jain, P.C. *et al, J. Am. Chem. Soc.*, 1967, **89**, 6131 (*cryst struct*)

$C_7H_{18}I_2NiOP_2$ IC-005801

Carbonyldiiodobis(trimethylphosphine)nickel, 9CI
Bis(*trimethylphosphine*)*carbonylnickel diiodide*
[35872-05-0]

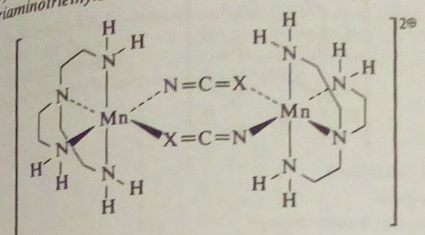


M 492.6
Dark-brown cryst. Fairly stable in solid state and in soln. under CO. Sol. C_6H_6, CH_2Cl_2, insol. EtOH. Solns. slowly dec. under inert atm., can be handled briefly in air.

Pankowski, M. *et al, J. Organomet. Chem.*, 1976, **110**, 331 (*synth, ir*)
Saint-Joly, C. *et al, Inorg. Chem.*, 1980, **19**, 2403 (*synth, struct*)

$C_7H_{18}MnN_5O^{\oplus}$ IC-005802

(Cyanato-*N*)[tris(2-aminoethyl)amine]manganese(*II*)(1+)
[N,N-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]
(*cyanato*-N)*manganese*(*1+*), *10CI. Isocyanato*(*2,2′,2″-triaminotriethylamine*)*manganese*(II)(*1+*)



X = O
dimer

M 243.1 (ion)
Dimeric cation. The ions $[MnXN(CH_2CH_2NH_2)_3]^{\oplus}$ (X = Cl, Br, CN, NCS, N_3) are also known.

Dimeric-form

Bis-μ-isocyanatobis(*2,2′,2″-triaminotriethylamine*)*dimanganese*(2+). *Bis*[N,N-*bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*bis*(*cyanato*-N)*dimanganese*(2+)
$C_{14}H_{36}Mn_2N_{10}O_2^{2\oplus}$ M 486.3 (ion)

Bis-tetraphenylborate: [64682-56-0].
$C_{62}H_{76}B_2Mn_2N_{10}O_2$ M 1124.8
Synth. by adding aq. solns. of the ligand, NaNCO and $NaBPh_4$ to aq. $MnSO_4.H_2O$ under N_2. Clear rectangular prisms (MeCN), stable in dry air. μ_{eff} = 4.85μ_B (296K).

Laskowski, E.J. *et al, Inorg. Chem.*, 1978, **17**, 457 (*synth, cryst struct, ir, magnetism, esr*)

$C_7H_{18}MnN_5S^{\ominus}$ IC-005803

(Thiocyanto-*N*)[tris(2-aminoethyl)amine]manganese(*II*)(1+)
[N,N-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]
(*thiocyanato*-N)*manganese*(*1+*), *10CI.*
Isothiocyanato(*2,2′,2″-triaminotriethylamine*)*manganese*(II)(*1+*)

As (Cyanato-*N*)[tris(2-aminoethyl)amine]manganese(*II*)(1+), IC-005802 with

X = S

M 259.2 (ion)
Dimeric cation. The ions $[MnXN(CH_2CH_2NH_2)_3]^{\oplus}$ (X = Cl, Br, CN, N_3, NCO) also known.

Dimeric-form

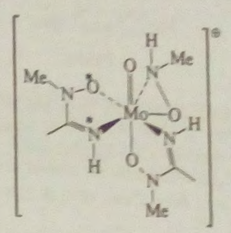
Bis(*isothiocyanato*)*bis*(*2,2′,2″-triaminotriethylamine*)*dimanganese*(2+). *Bis*[N,N-*bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]*bis*(*thiocyanato*-N)*dimanganese*(2+)
$C_{14}H_{36}Mn_2N_{10}S_2^{2\oplus}$ M 518.5 (ion)
Synth. by adding aq. solns. of the ligand, NaNCS and $NaBPh_4$ to $MnSO_4.H_2O$ in H_2O under N_2. μ_{eff} = 5.85μ_B (267K).

Bis-tetraphenylborate:
$C_{31}H_{38}BMnN_5S$ M 578.4
Clear rectangular prisms (MeCN), stable in dry air.

Laskowski, E.J. *et al, Inorg. Chem.*, 1978, **17**, 457 (*synth, cryst struct, ir, magnetism, esr*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 59 (*rev, bibl*)

$C_7H_{18}MoN_5O_4^{\oplus}$ IC-005804

Bis(*N*-hydroxy-*N*-methylacetamidinato-*N′,O*)(*N*-methylhydroxylamido-*N,O*)oxomolybdenum(*VI*)(1+)
(*N-Hydroxymethanaminato*-N,O)*bis*(*N-hydroxy-N-methylethanimidamidato*-N′,O)*oxomolybdenum*(VI)(*1+*), *10CI*



Major isomer
(*Minor isomer with • positions reversed*)

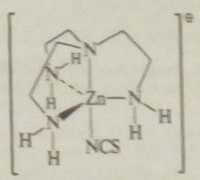
M 332.1 (ion)
Pentagonal bipyramidal. The bi-equatorial acetamidinato ligand coordinates as shown (75%) or in opposite fashion (25%).

Chloride: [79110-77-3].
Air-stable orange cryst. Sol. H_2O (dec.).
Perchlorate: [79356-01-7].
Orange cryst.

Wieghardt, K. *et al, Chem. Ber.*, 1981, **114**, 2700 (*cryst struct, synth, pmr*)

$C_7H_{18}N_5SZn^{\oplus}$ IC-005805

[Tris(2-aminoethyl)amine](thiocyanato-*N*)zinc(1+)
[N,N-*Bis*(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″,N‴]
(*thiocyanato*-N)*zinc*(*1+*), *9CI.* [*4*-(*2-Aminoethyl*)*diethylenetriamine*](*isothiocyanato*)*zinc*(*1+*). *β,β′,β″-Triaminotriethylamine*(*isothiocyanato*)*zinc*(*1+*)



M 269.7 (ion)
Trig. bipyramidal cation.

Thiocyanate: [21370-46-7].
White cryst.
Perchlorate: [59380-12-0].
White cryst. (H_2O). Sol. MeOH, MeCN, $EtNO_2$, DMF, DMSO; sl. sol. higher alcohols; insol. non-polar solvs.
▷ Potentially explosive.

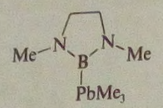
[34404-53-0, 59335-74-9]

Cayley, G.R. *et al, Trans. Faraday Soc.*, 1971, **67**, 2896 (*raman*)
Diaz, M. *et al, J. Inorg. Nucl. Chem.*, 1975, **37**, 2469 (*synth, ir, conductivity*)

$C_7H_{19}BN_2Pb$ IC-005806

1,3-Dimethyl-2-(trimethylplumbyl)-1,3,2-diazaborolidine, 9CI

[58747-16-3]



M 349.2

Trigonal boron compd. Synth. from Me_3PbBr with Li metal in THF at −78°, followed by addition of 2-chloro-1,3-dimethyl-1,3,2-diazaborolidine and warming to −10°. C_6H_6 soln. stable for several days at −10°.

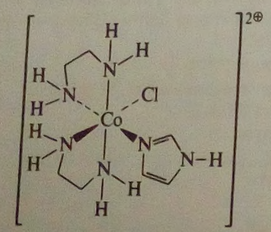
Kennedy, J.D. *et al*, *Inorg. Chem.*, 1976, **15**, 1299 (*nmr*)

$C_7H_{20}ClCoN_6^{2\oplus}$ IC-005807

Chlorobis(ethylenediamine)imidazolecobalt(*III*)(2+)

*Chlorobis(1,2-ethanediamine-*N,N′*)(1H-imidazole-*N^3*)cobalt*(III), *10CI*

[60314-38-7]



M 282.6 (ion)

Octahedral. Single Λ-*cis*-isomer formed.

Dichloride: [55190-25-5].

Brick-red cryst. + $\frac{1}{2}H_2O$. Sol. aq. $HClO_4$, probably with reaction.

[56906-96-8, 56906-97-9, 61004-29-3]

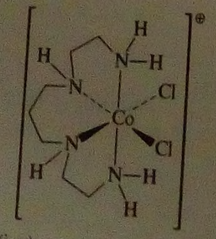
Kindred, F.J. *et al*, *Inorg. Chim. Acta*, 1975, **14**, 185 (*synth, uv, ord, cd*)

Zimmer-Gasser, B., *Inorg. Chim. Acta*, 1981, **55**, 43 (*cryst struct*)

Dash, K.C. *et al*, *J. Mol. Struct.*, 1981, **72**, 269 (*synth, ir, pmr, cmr*)

$C_7H_{20}Cl_2CoN_4^{\oplus}$ IC-005808

Dichloro(1,4,8,11-tetraazaundecane)cobalt(*III*)(1+)



cis-form

M 290.1 (ion)

cis-form

Chloride:

$C_7H_{20}Cl_3CoN_4$ M 325.5

Violet cryst. Sol. H_2O.

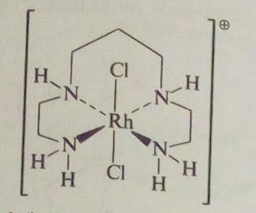
trans-form

Chloride: Green cryst. Sol. H_2O.

Bosnich, B. *et al*, *J. Chem. Soc. A*, 1966, 1331 (*synth, uv*)

$C_7H_{20}Cl_2N_4Rh^{\oplus}$

Dichloro(1,4,8,11-tetraazaundecane-N^1,N^4,N^8,N^{11})rhodium(*III*)(1+) IC-005809



trans-form

M 334.0 (ion)

trans-form

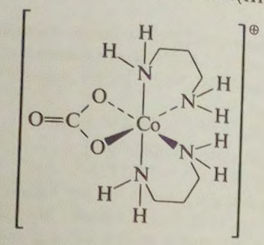
Nitrate: Yellow cryst.

Bosnich, B., *J. Chem. Soc. A*, 1966, 1331 (*synth, uv*)

$C_7H_{20}CoN_4O_3^{\oplus}$ IC-005810

(Carbonato)bis(1,3-propanediamine)cobalt(*III*)(1+), 8Cl

Carbonatobis(trimethylenediamine)cobalt(III)(*1+*)



M 267.1 (ion)

Perchlorate: [31188-12-2].

Deep red cryst.

▷ Potentially explosive.

Geue, R.J. *et al*, *J. Chem. Soc. A*, 1971, 2981 (*synth, cryst struct*)

$C_7H_{20}CoN_6^{3\oplus}$ IC-005811

Pentaammine(benzonitrile)cobalt(*III*)(3+)

[46343-53-7]

$[(H_3N)_5Co(NCPh)]^{3\oplus}$

M 247.2 (ion)

Triperchlorate: [38363-82-5].

Synth. from aquapentaamininecobalt(*III*) perchlorate, fivefold excess of benzonitrile, molecular sieve and trimethyl phosphate. Yellow-brown solid (H_2O). Sol. H_2O. $Ir_{C\equiv N}$ 2270 (2230) cm^{-1}.

▷ Potentially explosive.

Pinnell, D. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 6104 (*synth, uv, ir, pmr, kinetics*)

Ellis, W.R. *et al*, *Inorg. Chem.*, 1982, **21**, 834 (*reactions*)

$C_7H_{20}CoN_9^{2\oplus}$ IC-005812

Pentaammine(5-phenyl-1*H*-tetrazolato)cobalt(*III*)(2+), 11Cl

M 289.2 (ion)

Ligand can bond through any N.

N^1-bonded-form

Iodide: [79899-67-5].

Light-sensitive solid. Sol. H_2O, DMSO.

N^2-bonded-form

Iodide: [79899-69-7].

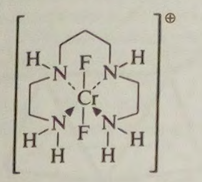
Light-sensitive solid. Sol. H_2O, DMSO.

Ellis, W.R. *et al*, *Inorg. Chem.*, 1982, **21**, 834 (*synth, uv, pmr*)

$C_7H_{20}CrF_2N_4^{\oplus}$ IC-005813

Difluoro(1,4,8,11-tetraazaundecane)chromium(*III*)(1+)

*[N,N′-Bis(2-aminoethyl)-1,3-propanediamine-*N,N′,N″,N‴*]difluorochromium(1+), 10CI, 8CI. (1,9-Diamino-3,7-diazanonane)difluorochromium*(III)(*1+*)



M 250.2 (ion)

Octahedral cation.

trans-form

The *meso* (*R,S*)-config. of the 2 inner asymmetric nitrogen ligands remains intact even in basic soln. Cr—F 185, 190, Cr—N_{av} 206 pm.

Perchlorate: [28294-85-1].

Synth. from ligand + *trans*-$[CrPy_4F_2]ClO_4$ in 2-methoxyethanol. Orange red cryst. (H_2O). λ_{max} 348, 453, 522 nm.

[69483-97-2]

Glerup, J. *et al*, *Acta Chem. Scand., Ser. A*, 1970, **24**, 247 (*synth, uv-vis*)

Bang, E. *et al*, *Acta Chem. Scand., Ser. A*, 1978, **32**, 833 (*cryst struct*)

$C_7H_{20}IrN_6^{3\oplus}$ IC-005814

Pentaammine(benzonitrile)iridium(*III*)(3+), 10CI

Pentaammine(phenyl cyanide)iridium(III)(*3+*)

$[Ir(NH_3)_5(NCPh)]^{3\oplus}$

M 380.4 (ion)

Octahedral cation.

Triperchlorate: [73453-87-9].

Sol. H_2O.

Foust, R.D. *et al*, *Inorg. Chem.*, 1972, **11**, 899 (*synth, ir, uv*)

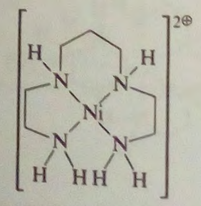
Talebinasab-sarvari, M. *et al*, *Inorg. Chem.*, 1980, **19**, 1835 (*synth, photochem, uv*)

$C_7H_{20}N_4Ni^{2\oplus}$ IC-005815

(1,4,8,11-Tetraazaundecane)nickel(*II*)(2+)

*[N,N′-Bis(2-aminoethyl)-1,3-propanediamine-*N,N′,N″,N‴*]nickel*(II)(*2+*), *8CI. (2,3,2-Tet)nickel*(*2+*)

[25669-75-4]



M 218.9 (ion)

Square planar. Forms 6 coordinate complexes with coordinating anions and partly in H_2O.

Diperchlorate: [27537-50-4].

$C_7H_{20}Cl_2N_4NiO_8$ M 417.8

Orange-yellow solid. Sol. H_2O, DMF, DMSO.

▷ Potentially explosive.

Diiodide: [15730-04-8].

$C_7H_{20}I_2N_4Ni$ M 472.7

Brown-red solid + $1H_2O$. Sol. H_2O.

Bosnich, B. *et al*, *J. Chem. Soc. A*, 1966, 1331 (*synth, uv*)

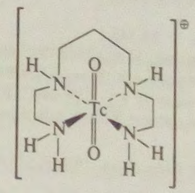
Curtis, N.F. *et al*, *Aust. J. Chem.*, 1974, **27**, 1167.

Cook, D.F. *et al*, *Inorg. Chim. Acta*, 1978, **31**, 59 (*synth, uv*)

$C_7H_{20}N_4O_2Tc^{\oplus}$ IC-005816

(1,9-Diamino-3,7-diazanonane)dioxotechnetium(*V*)(1+)

(1,4,8,11-Tetraazaundecane)dioxotechnetium(V)(*1+*). [N,N′-*Bis(2-aminoethyl)-1,3-propanediamine-*N,N′,N″,N‴*]dioxotechnetium(1+), 11CI. [2,3,2-Tet]dioxotechnetium*(V)(*1+*)



M 291.1 (ion)

Approx. octahedral cation. Prep. from $[TcOCl_4]^{\ominus}$ + ligand in THF.

Hexafluorophosphate: [97332-98-4].

Yellow solid.

Bläuenstein, P. *et al*, *Int. J. Appl. Radiat. Isot.*, 1985, **36**, 315 (*synth, ir, uv, chromatog, biodistribn*)

$C_7H_{20}N_5O_2Ru^{2\oplus}$ IC-005817

Pentaammine(benzoato-*O*)ruthenium(*III*)(2+)

$[Ru(NH_3)_5(OOCPh)]^{2\oplus}$

M 307.3 (ion)

Prepd. by oxidation of ruthenium(*II*) analogue. Readily reduced by standard reducing agents; undergoes a wide range of anation and aquation reactions.

Diperchlorate: [25590-48-1].

Yellow solid. Sol. H_2O.

▷ Potentially explosive.

Stritar, J.A. *et al*, *Inorg. Chem.*, 1969, **8**, 2281 (*synth, uv, reactions*)

Lin, S.-W. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 290 (*uv*)

Ohyoshi, A. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2121; 1973, **46**, 2431 (*reaction*)

Ohkubo, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 2651; 1975, **48**, 774 (*reactions*)

Ohyoshi, A. *et al*, *Chem. Lett.*, 1973, 737 (*electrochem*)

$C_7H_{20}N_6Rh^{3\oplus}$ IC-005818

Pentaammine(benzonitrile)rhodium(*III*)(3+), 9Cl

[46343-55-9]

$[Rh(NH_3)_5(NCPh)]^{3\oplus}$

M 291.1 (ion)

Triperchlorate: [36449-60-2].

White solid. Sol. H_2O.

▷ Potentially explosive.

Foust, R.D. *et al*, *Inorg. Chem.*, 1972, **11**, 899 (*synth, ir, uv*)

Zanella, A.W. *et al*, *Inorg. Chem.*, 1975, **14**, 700 (*hydrol, kinetics*)

$C_7H_{20}N_6Ru^{2\oplus}$ IC-005819

Pentaammine(benzonitrile)ruthenium(*II*)(2+), 9CI

[31418-68-5]

$[Ru(NH_3)_5N{\equiv}CPh]^{2\oplus}$

M 289.3 (ion)

Prep. by the treatment of Pentaammine(aqua) ruthenium(*II*)(2+), IC-019980 with PhC≡N, by the aerial oxidation of Pentaammine(benzylamine) ruthenium(*III*)(3+), IC-005832, or by treating Hexaammineruthenium(*III*)(3+), IC-020001 with PhCHO/$OH^{\ominus}$, followed by aerial oxidation. Sol. H_2O.

Dibromide:
$C_7H_{20}Br_2N_6Ru$ M 449.1
Yellow salt. Ir ν_{CN} 2194 cm^{-1} (KBr).

Diiodide:
$C_7H_{20}I_2N_6Ru$ M 543.1
Orange-yellow salt. Ir ν_{CN} 2190 cm^{-1} (nujol).

Diperchlorate: Yellow salt. Ir ν_{CN} 2188 cm^{-1} (KBr).

Bis-tetrafluoroborate: Ir ν_{CN} 2194 cm^{-1} (KBr).

Bis-hexafluorophosphate: Yellow salt. Ir ν_{CN} 2219 cm^{-1} (nujol).

Clarke, R.E. *et al*, *Inorg. Chem.*, 1970, **9**, 227 (*synth, ir, uv, reactions*)
Chatt, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1971, 3168 (*synth, ir*)
Allen, R.J. *et al*, *Inorg. Chem.*, 1972, **11**, 679 (*formn*)
Foust, R.D. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 5686 (*pmr*)
Chaisson, D.A. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 6665 (*photochem*)
Diamond, S.E. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 2661 (*synth, uv, electrochem*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*electrochem*)
Guengerich, C.P. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 3298 (*synth, ir, uv*)
Dowling, N. *et al*, *Inorg. Chem.*, 1981, **20**, 2345 (*electrochem*)

$C_7H_{20}N_6Ru^{3\oplus}$ IC-005820

Pentaammine(benzonitrile)ruthenium(*III*)(3+), 8CI

$[Ru(NH_3)_5N{\equiv}CPh]^{3\oplus}$

M 289.3 (ion)

Presumed octahedral. Prepd. by oxidation of Pentaammine(benzonitrile)ruthenium(*II*)(2+), IC-005819 with $Ag^{\oplus}$ or Ce(*IV*).

Tribromide: [27346-70-9].
Ir ν_{CN} 2268 cm^{-1} (KBr).

Tris-tetrafluoroborate: [21858-73-1].
Ir ν_{CN} 2272 cm^{-1} (KBr).

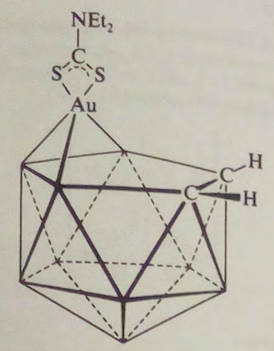
Triperchlorate: [27346-53-8].
Ir ν_{CN} 2267 cm^{-1} (KBr).

Clarke, R.E. *et al*, *Inorg. Chem.*, 1970, **9**, 227 (*synth, ir, uv*)

$C_7H_{21}AuB_9NS_2$ IC-005821

(Diethylcarbamodithioato-*S,S'*)(9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]gold, 10CI

[62572-50-3]



M 477.6

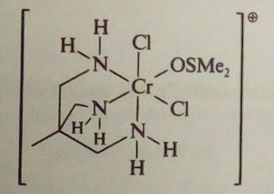
"Slipped" dicarbollide ligand in struct. Orange cryst. (CH_2Cl_2/pentane). Sol. CH_2Cl_2. Mp 115° dec.

Colquhoun, H.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 303 (*synth, cryst struct, nmr*)

$C_7H_{21}Cl_2CrN_3OS^{\oplus}$ IC-005822

Dichloro(dimethyl sulfoxide)[1,1,1-tris(aminomethyl) ethane]chromium(*III*)(1+)

*[2-(Aminomethyl)-2-methyl-1,3-propanediamine-*N,N',N"*] dichloro[sulfinylbis[methane]-*O*]chromium(1+), 10CI*



M 318.2 (ion)

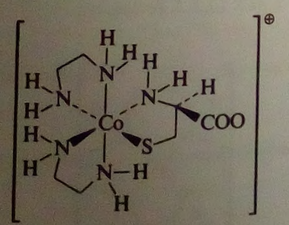
Octahedral complex, detailed struct. unknown. With H_2O gives dinuclear μ-hydroxo cations.

Iodide: [71480-22-3].
Violet cryst. + H_2O.

Wieghardt, K. *et al*, *Chem. Ber.*, 1979, **112**, 2837 (*synth*)

$C_7H_{21}CoN_5O_2S^{\oplus}$ IC-005823

[L-Cysteinato(2−)-*N,S*]bis(1,2-ethanediamine-*N,N'*) cobalt(*III*)(1+), 9CI



M 298.2 (ion)

Model complex for studies of reactions of metal-amino acid complexes.

Iodide: [25749-39-7].
Dark brown cryst. Sol. H_2O.

Perchlorate: [54713-70-1].

Brown cryst. (H_2O).
▷ Potentially explosive.

S-oxide: [54750-90-2]. (*Cysteinesulfenato-*N,S)*bis(ethylenediamine)cobalt*(III)(1+). *Bis(1,2-ethanediamine-*N,N')*[3-sulfeno-L-alaninato(2−)-*N,S*]cobalt*(III)(1+), *9CI*
$C_7H_{21}CoN_5O_3S^{\oplus}$ M 314.2 (ion)
Synth. by H_2O_2 oxidation of parent complex.

S-oxide, perchlorate: [54713-72-3].
Yellow cryst. (2-propanol aq.). Sol. H_2O.

S,S-dioxide: (*Cysteinesulfinato-*N,S)*bis(ethylenediamine) cobalt*(III)(1+). [*(2-Amino-2-carboxyethyl)sulfonyl-*N,S] *bis(1,2-ethanediamine-*N,N')*cobalt*(III)(1+), *9CI*
$C_7H_{21}CoN_5O_4S^{\oplus}$ M 330.2 (ion)

S,S-dioxide, perchlorate: [54750-89-9].
Synth. by oxidation of parent compd. with excess H_2O_2.
Yellow solid.

Kothari, V.M. *et al*, *Inorg. Chem.*, 1969, **90**, 561 (*synth, ir, elec cond*)
Sloan, C.P. *et al*, *Inorg. Chem.*, 1975, **14**, 1481 (*synth, ir, pmr, derivs*)

$C_7H_{21}CoN_6OS^{2\oplus}$ IC-005824

Pentaammine(*N*-phenylthiocarbamato-*S*)cobalt(*III*)(2+)

*Pentaammine(phenylcarbamothioato-*S*)colbalt*(III)(2+), *11CI*

$[(H_3N)_5CoSCONHPh]^{2\oplus}$

M 296.2 (ion)

Octahedral.

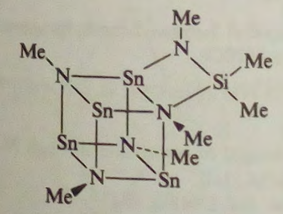
Diperchlorate: [82292-91-9].
Cryst. + $1H_2O$. Sol. DMSO.
▷ Potentially explosive.

Balahura, R.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 747 (*synth, cryst struct, pmr, uv*)

$C_7H_{21}N_5SiSn_4$ IC-005825

μ3-[Dimethylsilylbis(methylamido)]tris-μ3-(methylimido) tetratin

Tris[μ3-[methanaminato(2−)]][μ3-[N,N',1,1-tetramethylsilanediaminato(2−)-N:N:N']]tetratin, 10CI. 1,3,5,7,9,10,10-Heptamethyl-1,3,5,7-tetraazonia-10-sila-2λ3,4λ3,6λ3,8λ3-tetrastannatapentacyclo[4.2.2.0^{2,5}.0^{3,8}.0^{4,7}] decane



M 678.2

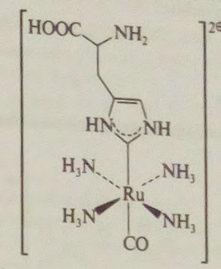
Orange cryst. Sol. hexane, Et_2O.

Veith, M. *et al*, *J. Organomet. Chem.*, 1981, **216**, 27 (*synth, pmr, cryst struct*)

$C_7H_{21}N_7O_3Ru^{2\oplus}$ IC-005826

Tetraammine(carbonyl)(histidine)ruthenium(*II*)(2+)

[4-(2-Amino-2-carboxyethyl)-1,3-dihydro-2H-imidazol-2-ylidene]-tetraamminecarbonylruthenium(II)(2+), *9CI*



M 352.3 (ion)

The histidine ligand is bound through C(2) as an ylid. Prepd. by reducing $[Ru(NH_3)_4(hist)Cl]^{2\oplus}$ with Zn/Hg, followed by CO. Sol. H_2O.

Diperchlorate: [50938-48-2].
Solid salt.

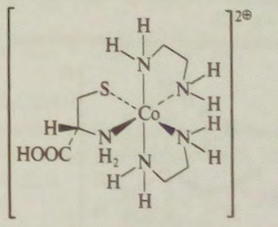
Sundberg, R.J. *et al*, *Bioinorg. Chem.*, 1973, **3**, 39 (*synth, uv, pmr, electrochem*)

$C_7H_{22}CoN_5O_2S^{2\oplus}$ IC-005827

Cysteinatobis(ethylenediamine)cobalt(*III*)(2+)

*(Cysteinato-*N,S)*bis(1,2-ethanediamine-*N,N')*cobalt*(III)(2+)

[63891-07-6]



R,Δ-*form*

M 299.2 (ion)

On oxidation forms a sulfenamide complex.

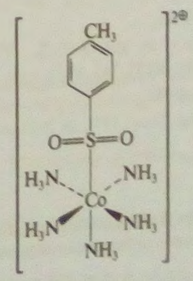
Diperchlorate: [66417-02-5].
Chocolate brown needles + $1H_2O$.

Jackson, W.G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1976, 934 (*struct*)
Gainsford, G.J. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 2383 (*synth, struct, resoln, uv-vis, reaction*)
Freeman, H.C. *et al*, *Inorg. Chem.*, 1978, **17**, 3513 (*synth*)

$C_7H_{22}CoN_5O_2S^{2\oplus}$ IC-005828

Pentaammine(*p*-toluenesulfonyl)cobalt(*III*)(2+)

[64715-11-3]



M 299.2 (ion)
Octahedral at Co with long Co—N *trans* to S (202.3 pm).

Diperchlorate: [64715-13-5].
Yellow brown cryst. + $1H_2O$ (Me_2CO/Et_2O). Sol. H_2O.
▷ Potentially explosive.

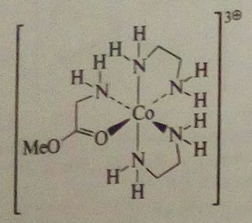
Elder, R.C. *et al, Inorg. Chem.*, 1978, **17**, 431 (*synth, cryst struct, kinetics*)

IC-005829

$C_7H_{23}CoN_5O_2^{3\oplus}$

Bis(ethylenediamine)(methyl glycinate)cobalt(*III*)(3+)

[22062-88-0]



M 268.2 (ion)
Triperchlorate: [17375-48-3].
No phys. props. reported.

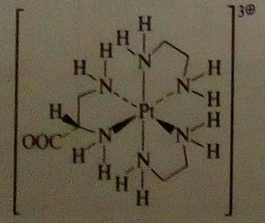
Buckingham, D.A. *et al, J. Am. Chem. Soc.*, 1967, **89**, 4539 (*pmr, ir*)
Clark, C.R. *et al, J. Am. Chem. Soc.*, 1981, **103**, 7023 (*synth*)

IC-005830

$C_7H_{23}N_6O_2Pt^{3\oplus}$

(3-Amino-L-alaninato-*N,N'*)bis(1,2-ethanediamine-*N,N'*) platinum(*IV*)(3+), 9Cl

2,3-Diaminopropionatobis(ethylenediamine)platinum(IV)



L-Alaninato-Δ-form

M 418.3 (ion)
Kinetically inert, enantiomers resolved. Synth. from *cis*-$[PtCl_2(en)_2]^{2\oplus}$ + diaminopropionic acid.

Δ-form

(+)-form
Less soluble form.

Hydrogen chloride (1:4): [60018-56-6].
White cryst. (dil. HCl). Sol. H_2O.

Λ-form

(−)-form
More soluble form.

Hydrogen chloride (1:4): [60018-57-7].
White cryst. (dil. HCl). Sol. H_2O.

[59982-44-4, 60018-55-5]

Liu, C.F. *et al, Inorg. Chem.*, 1976, **15**, 2415 (*synth, pmr, ord, cd, abs config, resol*)

IC-005831

$C_7H_{24}N_6Ru^{2\oplus}$

Pentaammine(benzylamine)ruthenium(*II*)(2+)

Pentaammine(benzenemethanamine)ruthenium(2+), 9Cl

$[(H_3N)_5RuNH_2CH_2Ph]^{2\oplus}$

M 293.3 (ion)
Sol. dil. HCl, H_2O.

Bis-hexafluorophosphate: [56082-84-9].
Synth. from Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 and benzylamine, followed by $[NH_4]PF_6$. Yellow solid (H_2O).

Diamond, S.E. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2661 (*synth, electrochem, oxidation*)

IC-005832

$C_7H_{24}N_6Ru^{3\oplus}$

Pentaammine(benzylamine)ruthenium(*III*)(3+)

Pentaammine(benzenemethanamine)ruthenium(3+), 9Cl

$[Ru(NH_3)_5NH_2CH_2Ph]^{3\oplus}$

M 293.3 (ion)

Tris-hexafluorophosphate: [56165-43-6].
Synth. by oxidising $[Ru(NH_3)_5(NH_2CH_2Ph)][PF_6]_2$ with aq. Br_2 or $Ag[OOCCF_3]$. White solid.

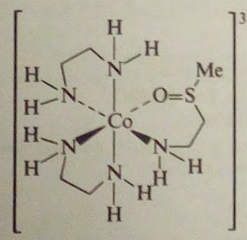
Diamond, S.E. *et al, J. Am. Chem. Soc.*, 1975, **97**, 2661 (*synth, electrochem*)

IC-005833

$C_7H_{25}CoN_5OS^{3\oplus}$

(Methyl 2-aminoethyl sulfoxide-*N,O*)bis(ethylenediamine) cobalt(*III*)(3+)

*Bis(1,2-ethanediamine-*N,N'*)[2-(methylsulfinyl)ethanamine-*N,O*]cobalt*(III)(3+), *11Cl*



M 286.3 (ion)
Unusual amine-sulfoxide ligand.
Triperchlorate: [80136-79-4].
Red powder. Sol. H_2O, $CHCl_3$.

Lydon, J.D. *et al, Inorg. Chem.*, 1982, **21**, 3180 (*synth, uv, ir, pmr*)

IC-005834

$C_7H_{26}CoN_6O_2^{3\oplus}$

Pentaammine(ethyl 2-cyano-2-methylpropanoate-*N*) cobalt(*III*)(3+), 10Cl

$[(H_3N)_5CoN{\equiv}CC(CH_3)_2COOEt]^{3\oplus}$

M 285.2 (ion)
Nitrile ester thought to coordinate through N.

Trinitrate: [78054-21-4].
Orange solid. Sol. DMSO, H_2O.

Greaser, I.I. *et al, J. Am. Chem. Soc.*, 1981, **103**, 3559 (*synth, ir, pmr*)

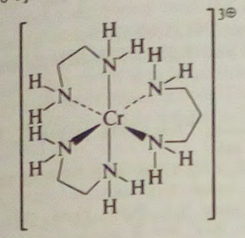
IC-005835

$C_7H_{29}CrN_6^{3\oplus}$

Bis(ethylenediamine)(1,3-propanediamine)chromium(*III*) (3+)

*Bis(1,2-ethanediamine-*N,N'*)(1,3-propanedamine-*N,N'*) chromium*(III)(3+), *11Cl, 10Cl, 9Cl*

[78404-06-5]



Λ-form

M 246.3 (ion)

Λ-form

(+)-form

Tribromide: Cryst. + H_2O.

(±)-form

Trichloride: [41101-32-0].
Yellow cryst. + H_2O (H_2O or aq. MeOH). V. sol. H_2O.
Dehydrates at 100-160°; deaminates at 190-230°.

Tribromide: [77056-59-8].
Yellow plates + $1H_2O$.

Trithiocyanate: [81194-09-4].
Yellow cryst. Deaminates at 50-135°.

[39023-34-2, 68223-83-6]

Rancke-Madsen, M. *et al, Acta Chem. Scand.*, 1972, **26**, 3405 (*synth, resoln*)
Duesler, E.N. *et al, Inorg. Chim. Acta*, 1978, **30**, 87 (*cryst struct, synth*)
McLean, J.A. *et al, Inorg. Chim. Acta*, 1981, **53**, L43 (*synth, bromide, uv-vis*)
Uehara, A. *et al, Inorg. Chem.*, 1982, **21**, 2422 (*synth, thermal dec*)

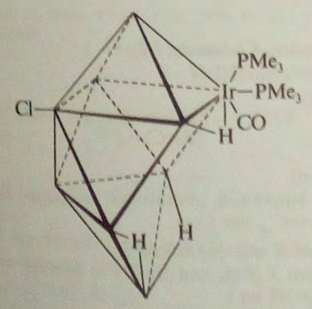
IC-005836

$C_7H_{28}B_8ClIrOP_2$

Chloro-2-carbonyl-2,2-bis(trimethylphosphine)-2-iridanonaborane

Carbonyl[(3,4,5,6-η)-4-chlorodecahydrooctaborato(3−)-H⁶] bis(trimethylphosphine)iridium, 11Cl

[96082-20-1]



M 504.4
nido-. Position of Cl variable. Air-stable v. pale yellow cryst. Sol. CH_2Cl_2.

[82472-61-5]

Bould, J. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2477 (*synth, pmr, B-11 nmr, P-31 nmr*)

IC-005837

$C_7H_{29}CoN_6^{3\oplus}$

Acetonitrilepentakis(methylamine)cobalt(*III*)(3+)

(Acetonitrile)pentakis(methanamine)cobalt(III)(3+), *11Cl*

$[Co(NH_2Me)_5(NCCH_3)]^{3\oplus}$

M 255.2 (ion)

Tris-trifluoromethanesulfonate: [100681-47-8].
Orange needles. Sol. H_2O.

Curtis, N.J. *et al, Inorg. Chem.*, 1986, **25**, 1033 (*synth, uv, pmr, kinetics*)

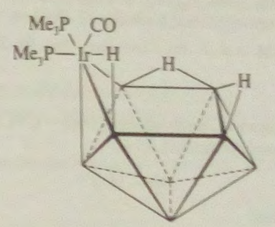
IC-005838

$C_7H_{29}B_8IrOP_2$

Carbonylbis(trimethylphosphine)[η⁴-undecahydrooctaborato(3−)-*H*]iridium, 11Cl

2-Carbonyl-2,2-bis(trimethylphosphine)-nido-2-iridanonaborane

[82497-54-9]



M 469.9
nido-. Pale-yellow cryst. (by chromatog. CH_2Cl_2/pet. ether). Sol. $CHCl_3$, CH_2Cl_2.

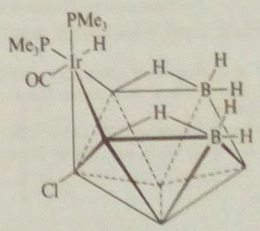
Bould, J. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2477 (*synth, cryst struct, B-11 nmr, P-31 nmr, pmr, ir*)

IC-005839

$C_7H_{30}B_8ClIrOP_2$

Carbonyl[η³-chloroundecahydrooctaborato(2−)] hydrobis(trimethylphosphine)iridium, 11Cl

[82458-33-1]



M 506.4
arachno-. Colourless cryst. (by chromatog.). Sol. CH_2Cl_2. Mp 140-150°.

Bould, J. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1903 (*synth, cryst struct, B-11 nmr, pmr, P-31 nmr, ir, ms*)

IC-005840

$C_7H_{31}CoN_5OS^{3\oplus}$

(Dimethylsulfoxide)pentakis(methylamine)cobalt(*III*)(3+)

Pentakis(methanamine)[sulfinylbis[methane]-O]cobalt(III) (3+), *11Cl*

$[Co(NH_2Me)_5(O{=}SMe_2)]^{3\oplus}$

M 292.3 (ion)

Tris-trifluoromethanesulfonate: [100681-49-0].

Purple solid. Sol. H_2O.

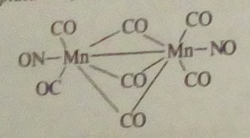
Curtis, N.J. *et al. Inorg. Chem.*, 1986, **25**, 1033 (*synth, uv, pmr, kinetics*)

IC-005841

$C_7Mn_2N_2O_9$

Tri-μ-carbonyltetracarbonyldinitrosyldimanganese

Dinitrosylheptacarbonyldimanganese



M 365.9

Struct. uncertain; analogue of $Fe_2(CO)_9$. Synth. by photolysis of $Mn(NO)(CO)_4$. Air-sensitive deep-red cryst. Subl.$_{0.1}$ 25°. Ir ν_{CO} 2101w, 2042vs, 2006vs, 1995w,sh, 1976s; ν_{CO}/ν_{NO} 1743m, 1735m,1731w, 1726w, 1710m cm^{-1} (1,2-dichloroethane). Dec. *ca.* 140°.

Treichel, P.M. *et al. J. Am. Chem. Soc.*, 1961, **83**, 2593 (*synth, ir*)

IC-005842

$C_7MoN_7^{5\ominus}$

Heptakis(cyano-*C*)molybdenum(*II*)(5−), 9Cl

Heptacyanomolybdate(II), (*5*−)

$[Mo(CN)_7]^{5\ominus}$

M 278.0 (ion)

Pentagonal bipyramidal at Mo.

Penta-Na salt: [64233-61-0].

Synth. by reaction of a mixture of MoO_3, NaOH, NaCN in H_2O, with H_2S. Cryst. $+5H_2O$; decahydrate also known. Diamagnetic.

Penta-K salt: [59433-33-9]. *Pentapotassium heptakis(cyano-C)molybdenum*(II), *hydrate. Potassium heptacyanomolybdate*(II), *hydrate*

Synth. by reaction of a mixture of MoO_3, KOH, KCN in H_2O, with H_2S. Yellow cryst. $+1H_2O$ (H_2O). Diamagnetic.

[64234-25-9]

Drew, M.G.B. *et al. Angew. Chem., Int. Ed. Engl.*, 1976, **88**, 855 (*deriv*)

Kiernan, P.M. *et al. Inorg. Nucl. Chem. Lett.*, 1976, **12**, 377 (*deriv*)

Drew, M.G.B. *et al. J. Chem. Soc., Dalton Trans.*, 1977, 1071; 1979, 1213 (*deriv*)

Mockford, M.J. *et al. Transition Met. Chem.*, 1984, **9**, 40 (*deriv*)

Mockford, M.J. *et al. J. Chem. Soc., Dalton Trans.*, 1985, 717 (*deriv*)

$C_7MoN_7^{4\ominus}$ **IC-005843**

Heptakis(cyano-*C*)molybdate(*III*)(4−), 11Cl

[35184-78-2]

$[Mo(CN)_7]^{4\ominus}$

M 278.0 (ion)

Anion has pentagonal bipyramidal struct. in aq. soln., in K_4 salt, anhyd., in Cs_4 salt, hydrate and in NaK_3 salt, dihydrate; thought to have monocapped trigonal prismatic struct. in K_4 salt, dihydrate by ir, Raman and x-ray diffraction comparisons. μ_{eff} = 1.84 (298K) (aq. soln.).

Tetra-K salt: [97332-62-2].

Obt. by heating dihydrate. Solid, dec. in air. Sol. H_2O, slowly sol. ethylene glycol; insol. common org. solvs. μ_{eff} = $1.08\mu_B$ (296K).

Tetra-K salt, dihydrate: [37838-58-7].

Synth. from K_3MoCl_6 and KCN. Dark green solid (EtOH aq.), dec. in air. Sol. H_2O, slowly sol. ethylene glycol; insol. common org. solvs. μ_{eff} = $1.80\mu_B$ (297K).

Tri-K, Na salt, dihydrate: [75446-13-8].

Synth. from $Na_5[Mo(CN)_7].10H_2O$, NaCN and KBH_4 or K_3MoCl_6 and NaCN. Dark green cryst., not isomorphous with K_4 salt, dihydrate. μ_{eff} = $1.78\mu_B$ (298K).

Tetra-Cs salt hydrate: [37838-60-1].

Synth. from CsCl and $K_4[Mo(CN)_7].2H_2O$. Dark green powder.

[37838-59-8]

Rossman, G.R. *et al. Inorg. Chem.*, 1973, **12**, 824 (*synth, ir, raman, esr, uv, K salts, Cs, salt*)

Hursthouse, M.B. *et al. Inorg. Chim. Acta*, 1980, **45**, L81 (*cryst struct, synth, esr, ir, raman, NaK_3 salt*)

Soares, A.M. *et al. J. Chem. Soc., Dalton Trans.*, 1981, 1886 (*synth, ir, raman, esr, NaK_3 salt, K salt*)

$C_7MoN_7^{3\ominus}$ **IC-005844**

Heptakis(cyano-*C*)molybdenum(*IV*)(3−), 9Cl

Heptacyanomolybdate(IV)(*3*−)

$[Mo(CN)_7]^{3\ominus}$

M 278.0 (ion)

Pentagonal bipyramidal at Mo.

Tri-Li salt: [116219-08-0].

Tri-Na salt: [116188-35-3].

$C_7MoN_7Na_3$ M 347.0

Other alkali metal salts are similar.

Vretsena, N.B. *et al. Koord. Khim.*, 1988, **14**, 855; *CA.* **109**, 121577w (*derivs*)

$C_7MoN_7^{2\ominus}$ **IC-005845**

Heptakis(cyano-*C*)molybdate(*V*)(2−), 10Cl

Heptacyanomolybdate(V)(*2*−)

[72330-05-3]

$[Mo(CN)_7]^{2\ominus}$

M 278.0 (ion)

Pentagonal bipyramidal at Mo (?). Obt. from photolysis of $[Mo(CN)_8]^{3\ominus}$ in MeOH. Paramagnetic.

Rehorek, D. *et al. Inorg. Chim. Acta*, 1979, **37**, L471 (*synth, esr*)

$C_7N_7Re^{4\ominus}$ **IC-005846**

Heptakis(cyano-*C*)rhenate(*III*)(4−)

Heptacyanorhenate(III)(*4*−)

[67462-54-8]

$[Re(CN)_7]^{4\ominus}$

M 368.3 (ion)

Pentagonal bipyramid; interatomic distances: Re—C_{ax} 207.7, Re—C_{eq} 209.5 pm.

Tri-Na, mono-K salt: [69350-06-7].

Synth. from K_2ReI_4 and NaCN in MeOH. Cryst. + $3H_2O$ (MeOH aq.).

Tetra-K salt: [73432-43-6].

Synth. from (i) $ReCl_3$ and KCN aq. in air (ii) K_2ReI_4 and KCN in MeOH. Pale yellow cryst. + $2H_2O$ (MeOH aq.). Diamagnetic.

Griffith, W.P. *et al. J. Chem. Soc., Dalton Trans.*, 1978, 1411 (*synth, ir, raman, struct*)

Manoli, J.-M. *et al. J. Chem. Soc., Dalton Trans.*, 1980, 192 (*cryst struct*)

$C_7N_7S_7Tc^{4\ominus}$ **IC-005847**

Heptakis(thiocyanato-*N*)technetate(*III*)(4−)

Heptaisothiocyanatotechnetate(III)(*4*−)

$[Tc(NCS)_7]^{4\ominus}$

M 505.4 (ion)

There has been controversy over the nature of thiocyanato-technetium(*III*) complexes - see also Hexakis(thiocyanato-*N*)technetate(*III*)(3−), IC-005626; no recent support for this heptathiocyanato species. Prep. by hydrazine reduction of $Tc(NCS)_6^{2\ominus}$ in MeOH (excess $NCS^{\ominus}$). V. easily oxidised. Paramagnetic; CT band at 410 nm.

Tetrakis-tetrabutylammonium salt: [72043-38-0].

Lemon yellow cryst.

Trop, H.S. *et al. J. Labelled Compd. Radiopharm.*, 1979, **16**, 82 (*synth, uv, electrochem*)

Jones, A.G. *et al. Int. J. Appl. Radiat. Isot.*, 1982, **33**, 867.

$C_7N_7Tc^{4\ominus}$ **IC-005848**

Heptakis(cyano-*C*)technetate(*III*)(4−), 10Cl

Heptacyanotechnetate(III)(*4*−)

$[Tc(CN)_7]^{4\ominus}$ (D_{5h})

M 281.0 (ion)

Pentagonal bipyramidal in solid and in soln. Synth. from $TcI_6^{2\ominus}$ by refluxing with KCN in MeOH under N_2. Aq. solns. are air-sensitive, giving $[TcO(CN)_5]^{2\ominus}$.

Tetra-K salt: [73396-81-3].

Yellow-orange cryst. $+2H_2O$. Diamagnetic.

Trop, H.S. *et al. Inorg. Chem.*, 1980, **19**, 1993 (*synth, uv, ir, magnetism*)

$C_7N_7Ti^{4\ominus}$ **IC-005849**

Heptakis(cyano-*C*)titanate(*III*)(4−), 10Cl

Heptacyanotitanate(III)

$[Ti(CN)_7]^{4\ominus}$

M 230.0 (ion)

Tetra-Cs salt: [75520-95-5].

$C_7Cs_4N_7Ti$ M 761.6

Synth. from $TiBr_3$ and CsCN in liq. NH_3. Grey-green solid. Paramagnetic, μ_{eff} = $1.69\mu_B$.

Nicholls, D. *et al. Inorg. Chim. Acta*, 1980, **41**, 233 (*synth, ir, uv-vis, magnetism*)

$C_7N_7V^{4\ominus}$ **IC-005850**

Heptakis(cyano-*C*)vanadate(*III*)(4−), 11Cl

[52163-66-3]

$[V(CN)_7]^{4\ominus}$

M 233.0 (ion)

Pentagonal bipyramidal, the angle C_{ax}—V—C_{ax} is 171° but all V—C dists. are the same.

Tetra-K salt: [53307-30-5].

Synth. by mixing aq. solns. of VCl_3 and KCN. Deep red solid + $2H_2O$ (MeOH/5% aq. KCN).

[38702-86-2]

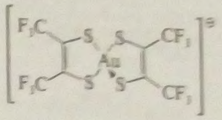
Levenson, R.A. *et al. Inorg. Chem.*, 1974, **13**, 105, 2761 (*synth, cryst struct, ir, raman, esr*)

Soares, A.M. *et al. J. Chem. Soc., Dalton Trans.*, 1981, 1886 (*synth*)

$C_8AuF_{12}S_4^{\ominus}$ **IC-005851**

Bis[*cis*-1,2-bis(trifluoromethyl)ethene-1,2-dithiolato]aurate(*I*)(1−)

Bis[1,1,1,4,4,4-hexafluoro-2-butene-2,3-dithiolato(2−)]aurate(1−), 8Cl



M 649.2 (ion)

Originally formulated as a five coordinate compd.

Ph_3PCl salt: [19562-28-8].

Pale green cryst. (CH_2Cl_2/pentane). Mp 140-142°.

[15008-60-3, 22239-86-7]

Davison, A. *et al. Inorg. Chem.*, 1967, **6**, 458 (*synth*)

Eisenmark, J.H. *et al. Inorg. Chem.*, 1968, **7**, 2636 (*cryst struct*)

Balch, A.L. *et al. Inorg. Chem.*, 1971, **10**, 388 (*reactions*)

$C_8AuN_4S_4^{2\ominus}$ **IC-005852**

Bis(maleonitriledithiolato)aurate(*II*)(2−)

Bis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S']aurate(2−), 10Cl

As Bis(maleonitriledithiolato)aurate(1−), IC-005853 with

n = 2

M 477.3 (ion)

Bis-tetrabutylammonium salt: [33637-83-1].

Light green cryst. (THF/MeOH). Paramagnetic: μ_{eff} = $1.85\mu_B$.

Waters, J.H. *et al. J. Am. Chem. Soc.*, 1965, **87**, 3534 (*synth*)

Waters, J.H. *et al. J. Chem. Soc., Chem. Commun.*, 1971, 834 (*synth, esr*)

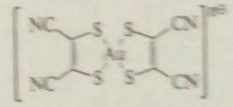
Viegers, T.P.A. *et al. Hyperfine Interact.*, 1978, **4**, 813 (*esr, mössbauer*)

$C_8AuN_4S_4^{\ominus}$ **IC-005853**

Bis(maleonitriledithiolato)aurate(1−)

Bis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S']aurate(1−), 10Cl

[14896-06-1]



n = 1

M 477.3 (ion)

Et_4N salt: Lustrous red brown needles (Me_2CO/1-propanol).

Tetrabutylammonium salt: [14710-21-5].

Red brown cryst. (Me_2CO/EtOH). Mp 174°.

Bis(triphenylphosphine)gold(1+) salt: [35925-82-1].

$C_{80}H_{68}Au_3N_4P_2S_4$ M 1198.8

Brown cryst. (THF). Mp > 250°.

Bis(triphenylarsine)gold(1+) salt:

$C_{80}H_{68}As_2Au_2N_4S_4$ M 1286.7

Red brown cryst. (THF). Mp 175°.

Davison, A. *et al. Inorg. Chem.*, 1963, **2**, 1227 (*synth*)

Noordik, J.H. *et al. J. Coord. Chem.*, 1973, **2**, 185 (*synth*)

Viegers, T.P.A. *et al. Hyperfine Interact.*, 1978, **4**, 813 (*mössbauer*)

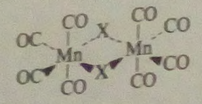
IC-005854

$C_8Br_2Mn_2O_8$

Di-μ-bromooctacarbonyldimanganese, 9CI, 8CI

Octacarbonyldi-μ-bromodimanganese

[18535-44-9]



X = Br

M 493.7

Synth. by heating $MnBr(CO)_5$ in pet. ether at 100-120°. Brown cryst. (C_6H_6 or CCl_4). Subl. 150°. Converted by CO into Bromopentacarbonylmanganese, IC-004608.

Monomer: Bromotetracarbonylmanganese

C_4BrMnO_4 M 246.8

Has no separate existence.

Abel, E.W. *et al, J. Chem. Soc.*, 1959, 1501 (*synth, props*)
Dahl, L.F. *et al, Acta Crystallogr., Sect. B*, 1963, **16**, 611 (*cryst struct*)
Farona, M.F. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1814 (*synth*)
Abel, E.W. *et al, Trans. Faraday Soc.*, 1967, **63**, 45 (*ir*)
Bamford, C.H. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1846 (*synth, ir*)

IC-005855

$C_8Br_2O_8Os_2$

Dibromooctacarbonyldiosmium, 8CI

[25685-07-8]

$BrOs(CO)_4$—$Os(CO)_4Br$

M 764.2

Diaxial. Synth. from $Os_2(CO)_8H_2$ and CBr_4 in heptane. Pale-yellow prisms (heptane). Mp 121-126° dec.

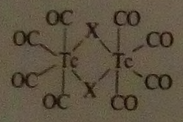
Moss, J.R. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 89 (*synth, ir, ms*)
Keiland, J.W. *et al, J. Organomet. Chem.*, 1978, **149**, 185 (*use*)

IC-005856

$C_8Br_2O_8Tc_2$

Di-μ-bromooctacarbonylditechnetium

[20468-83-1]



X = Br

M 581.7

Thought to have bridged struct. shown. Air-stable colourless cryst.

Hileman, J.C. *et al, Inorg. Chem.*, 1962, **1**, 933 (*synth, ir*)
El-Sayed, M.A. *et al, Inorg. Chem.*, 1963, **2**, 158 (*ir*)
Orgel, L.E., *Inorg. Chem.*, 1964, **3**, 303 (*ir*)

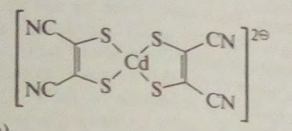
IC-005857

$C_8CdN_4S_4^{2\ominus}$

Bis(maleonitriledithiolato)cadmate(2−)

Bis(1,2-dicyanoethene-1,2-dithiolato-S,S′)cadmate(2−). Bis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S′] cadmate(2−), 9CI

[59982-86-4]



M 392.7 (ion)

Bis-Et_4N salt: [59982-87-5].
Cryst. (MeOH). Sol. DMSO.

Bis-tetrabutylammonium salt: [97251-92-8].
Cryst.

1,1′-Dimethyl-4,4′-bipyridinium(2+) salt: [107769-63-1].
Brown cryst. Sol. DMSO. Mp 273°.

Haberkorn, R.A. *et al, Inorg. Chem.*, 1976, **15**, 2408 (*synth, Cd-113 nmr, Et_4N salt*)
Fernandez, A. *et al, Chem. Ber.*, 1984, **117**, 3102; 1985, **118**, 1936 (*uv, photochem, Bu_4N salt*)
Kisch, H. *et al, Sci. Pap. Inst. Phys. Chem. Res. (Jpn.)*, 1984, **78**, 175 (*phosphorescence, fluorescence, Bu_4N salt*)
Lahner, S. *et al, Chem. Ber.*, 1987, **120**, 1011 (*synth, uv, dimethylbipyridinium salt*)

IC-005858

$C_8CdN_{12}^{2\ominus}$

Tetrakis(carbonimidoyl cyanamidato)cadmate(2−)

Tetrakis(dicyanamido)cadmate(2−)

$[Cd(NCNCN)_4]^{2\ominus}$

M 376.5 (ion)

Bis-Ph_4P salt: [107102-27-2].
Colourless cryst. (Me_2CO). Mp 182°.

Bis-Ph_4As salt: [107087-51-4].
Colourless cryst. (Me_2CO). Mp 162°.

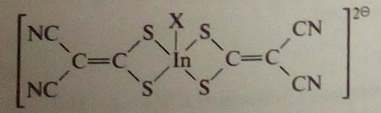
Köhler, H. *et al, Z. Anorg. Allg. Chem.*, 1986, **542**, 59 (*synth, ir, N-15 nmr, cmr, esca*)

IC-005859

$C_8ClInN_4S_4^{2\ominus}$

Chlorobis(1,1-dicyanoethylene-2,2-dithiolato)indate(2−)

Chlorobis[(dimercaptomethylene)malononitrilato(2−)] indate(2−), 8CI



X = Cl

M 430.6 (ion)

Bis-tetrabutylammonium salt: [31871-39-3].
From $InCl_3$, $Na_2[S_2C{=}C(CN)_2]$ and $[Bu_4N]Cl$ in MeOH. Pale yellow cryst. (MeOH). Mp 164°. Related compds. with X = Br or I also descr.

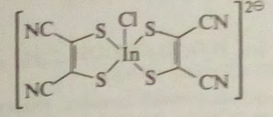
Tuck, D.G. *et al, J. Chem. Soc. A*, 1971, 214 (*synth, ir*)

IC-005860

$C_8ClInN_4S_4^{2\ominus}$

Chlorobis(maleonitriledithiolato)indate(2−)

Chlorobis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S′] indate(2−). Chlorobis(1,2-dicyanoethylene-1,2-dithiolato) indate(2−)



M 430.6 (ion)

Bis-Et_4N salt: [38333-72-1].
Synth. from $Na_2[InCl(S_2C_2(CN)_2)_2]$, $InCl_3$ and $[Et_4N]Cl$ in MeOH. Yellow moisture-sensitive cryst. (EtOH). Mp 148°.

Bis-tetrabutylammonium salt: [80996-33-4].
Synth. from $Na_2[InCl(S_2C_2(CN)_2)_2]$, $InCl_3$ and $[Bu_4N]Cl$ in MeOH. Yellow moisture-sensitive cryst. (MeOH/THF).

Fields, R.O. *et al, Inorg. Chem.*, 1971, **10**, 2808 (*synth*)
Allen, C.W. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 1951 (*ir*)
Day, R.O. *et al, Inorg. Chem.*, 1982, **21**, 2379 (*synth, cryst struct*)

IC-005861

$C_8Cl_2Mn_2O_8$

Octacarbonyldi-μ-chlorodimanganese, 9CI, 8CI

Di-μ-chlorooctacarbonyldimanganese

[18535-43-8]

As Di-μ-bromooctacarbonyldimanganese, IC-005854 with

X = Cl

M 404.8

Synth. by heating $MnCl(CO)_5$ in pet. ether at 100-120°.

Monomer: Tetracarbonylchloromanganese.
Chlorotetracarbonylmanganese

C_4ClMnO_4 M 202.4

Has no separate existence.

Abel, E.W. *et al, J. Chem. Soc.*, 1959, 1501 (*synth, props*)
El Sayed, M.A. *et al, Inorg. Chem.*, 1963, **2**, 158 (*ir*)
Zingales, F. *et al, Inorg. Chem.*, 1967, **6**, 1243 (*props*)
Farona, M.F. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1814 (*synth*)
Bamford, C.H. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1846 (*synth*)

IC-005862

$C_8Cl_2O_8Os_2$

Octacarbonyldichlorodiosmium, 8CI

[25685-06-7]

$ClOs(CO)_4$—$Os(CO)_4Cl$

M 675.3

Diaxial. V. pale-yellow prisms (heptane). Mp 118° dec.

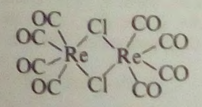
Moss, J.R. *et al, Inorg. Chem.*, 1977, **16**, 75.
Moss, J.R. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 89 (*synth, ir, ms*)

IC-005863

$C_8Cl_2O_8Re_2$

Octacarbonyldi-μ-chlorodirhenium, 10CI

[15189-52-3]



M 667.4

Synth. from $Re_2(CO)_{10}$ and Cl_2. Off-white cryst. Ir ν_{CO} 2114w, 2032s, 2000m, 1959m cm^{-1} (CCl_4).

IC-005864

$C_8Cl_2O_8Tc_2$

Octacarbonyldi-μ-chloroditechnetium

[20347-10-8]

As Di-μ-bromooctacarbonylditechnetium, IC-005856 with

X = Cl

M 492.8

Air-stable colourless cryst.

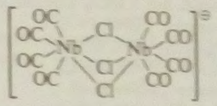
Hileman, J.C. *et al, Inorg. Chem.*, 1962, **1**, 933 (*synth, ir*)
El-Sayed, M.A. *et al, Inorg. Chem.*, 1963, **2**, 158 (*ir*)
Orgel, L.E., *Inorg. Chem.*, 1964, **3**, 303 (*ir*)

IC-005865

$C_8Cl_2Nb_2O_8^{\ominus}$

Octacarbonyltri-μ-chlorodiniobate(*1*)(1−)

Tri-μ-chlorobis[tetracarbonylniobium(I)](1−)



M 516.2 (ion)

Alkoxo bridged spp. obt. by metathetical exchange.

H compd.:
$C_8HCl_2Nb_2O_8$ M 517.2
Synth. by reaction of $Na[Nb(CO)_6]$.THF with dry HCl in heptane. Ochre cryst. + 2THF (THF/heptane). Sol. THF. Ir ν_{CO} 2023, 1910 cm^{-1} (toluene).

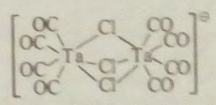
Calderazzo, F. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1989 (*synth, cryst struct, ir*)

IC-005866

$C_8Cl_2O_8Ta_2^{\ominus}$

Octacarbonyltri-μ-chloroditantalate(*1*)(1−)

Tri-μ-chlorobis(tetracarbonyltantalate(I))(1−)



M 692.3 (ion)

H compd., bis-THF complex:
$C_{16}H_{17}Cl_2O_{10}Ta_2$ M 837.5
Synth. by reaction of $Na[Ta(CO)_6]$.THF with dry HCl in heptane. Brown; not isol. in pure state. Sol. THF. Ir ν_{CO} 2010, 1895 cm^{-1} (toluene).

Calderazzo, F. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1989 (*synth, ir*)

IC-005867

$C_8Cl_6O_8Ru_2Si_2$

Octacarbonylbis(trichlorosilyl)diruthenium(*I*), 9CI

[25929-57-1]

Cl_3Si—$Ru(CO)_4$—$Ru(CO)_4$—$SiCl_3$ (*diax.*)

M 695.1

Synth. by the photolysis of $Ru_3(CO)_{12}$ in hexane in the presence of $SiCl_3H$. Pale yellow, air-sensitive cryst. Sol. hydrocarbon solvs. Mp 145-150°. Ir ν_{CO} 2086, 2056, 2050 cm^{-1} (cyclohexane).

Knox, S.A.R. *et al*, *J. Chem. Soc. A*, 1969, 2559 (*synth, ir*)
Ash, M.J. *et al*, *J. Chem. Soc. A*, 1971, 458 (*reaction*)
Van Buuren, G.N. *et al*, *Inorg. Chem.*, 1981, **20**, 4361.
Pomeroy, R.K. *et al*, *Can. J. Chem.*, 1982, **60**, 1279 (*synth*)
Krentz, R. *et al*, *Inorg. Chem.*, 1985, **24**, 2976 (*Si-29 nmr*)

$C_8Cl_{12}O_8Th$ IC-005868

Thorium(*IV*) trichloroacetate

Tetrakis(*trichloroacetato*-O,O′)*thorium*(IV)

$Th(OCOCCl_3)_4$

M 881.5
Usually obtd. as a hydrate. Mp 210° dec. Yields $ThCl_4$ at 260-340°; $ThOCl(OCOCCl_3)$ in air. Forms wide range of Lewis base adducts.

Monohydrate: [90189-26-7].
$C_8H_2Cl_{12}O_9Th$ M 899.5
Colourless cryst. Sol. H_2O. Loses H_2O in range 120-140°.

Tris-N,N-*dimethylacetamide complex:* [60447-62-3].
$C_{20}H_{27}Cl_{12}N_3O_{11}Th$ M 1142.9
Colourless solid. Sol. $CHCl_3$. Dec. on keeping.

Tris-DMSO complex: [88006-19-3].
$C_{14}H_{18}Cl_{12}O_{11}S_3Th$ M 1115.9
White solid. Sol. CH_2Cl_2, $CHCl_3$.

Bis-Ph_3SO complex: [88006-25-1].
$C_{32}H_{20}Cl_{12}O_{10}S_2Th$ M 1286.1
White solid. Sol. CH_2Cl_2, $CHCl_3$.

Bis-Py complex: [74594-60-8].
White solid.

Bis-Py N-*oxide complex:* [74594-62-0].
$C_{18}H_{10}Cl_{12}N_2O_{10}Th$ M 1071.7
White solid.

Tetrakis-Me_3PO complex: [88006-11-5].
$C_{20}H_{36}Cl_{12}O_{12}P_4Th$ M 1249.8
White solid. Sol. CH_2Cl_2.

Tris-Me_2PhPO complex: [93366-28-0].
$C_{32}H_{33}Cl_{12}O_{11}P_3Th$ M 1343.9
White solid. Sol. CH_2Cl_2.

Tris-Ph_2MePO complex: [93366-32-6].
$C_{47}H_{39}Cl_{12}O_{11}P_3Th$ M 1530.2
White solid. Sol. CH_2Cl_2, THF.

Tris-Ph_3PO complex: [88027-33-2].
$C_{62}H_{45}Cl_{12}O_{11}P_3Th$ M 1716.4
White solid. Sol. CH_2Cl_2.

Tetrakis-N,N′-*dimethylurea complex:* [93366-24-6].
$C_{20}H_{32}Cl_{12}N_8O_{12}Th$ M 1233.9
White solid. Sol. CH_2Cl_2.

Gelecenau, I. *et al*, *Radiokhimiya*, 1964, 693 (*synth*)
Bagnall, K.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1109; 1983, 1153 (*synth, complexes, ir*)
Malhotra, K.C. *et al*, *Indian J. Chem., Sect. A*, 1979, **18**, 423 (*synth, complexes*)
Matveev, Yu.S. *et al*, *Koord. Khim.*, 1983, **9**, 361; 1984, **10**, 511 (*synth, ir, tga*)
Ahmed, I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 1527 (*complexes, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 44, *Suppl.*, 1985, **E**, 12, 52, 69; *Suppl. vol.*, 1988, **C7**, 58 (*rev*)

$C_8Cl_{12}O_8U$ IC-005869

Uranium(*IV*) trichloroacetate

Tetrakis(*trichloroacetato*-O,O′)*uranium*

[10045-01-9]

$U(OCOCCl_3)_4$

M 887.5
Green solid. Sol. H_2O, Et_2O, EtOH, C_6H_6. $\mu_{eff} = 3.32\mu_B$. Dec. >150° affording $UOCl_2$.

Tris-N,N-*dimethylacetamide complex:* [60447-64-5].
$C_{20}H_{27}Cl_{12}N_3O_{11}U$ M 1148.9
Green solid. Sol. $CHCl_3$. Dec. on keeping.

Tetrakis-N,N′-*dimethylurea:* [93366-25-7].
$C_{20}H_{32}Cl_{12}N_8O_{12}U$ M 1239.9
Green solid. Sol. CH_2Cl_2.

Tris-DMSO complex: [88006-20-6].
$C_{14}H_{18}Cl_{12}O_{11}S_3U$ M 1121.9
Green solid. Sol. CH_2Cl_2, $CHCl_3$.

Tris-Ph_2SO complex: [88006-26-2].
$C_{44}H_{30}Cl_{12}O_{11}S_3U$ M 1494.3
Green solid. Sol. CH_2Cl_2, $CHCl_3$.

Tetrakis-Me_3PO complex: [88027-32-1].
$C_{20}H_{36}Cl_{12}O_{12}P_4U$ M 1255.8
Green solid. Sol. CH_2Cl_2, $CHCl_3$.

Tris-Me_2PhPO complex: [93366-29-1].
$C_{32}H_{33}Cl_{12}O_{11}P_3U$ M 1349.9
Green solid. Sol. CH_2Cl_2.

Tris-Ph_2MePO complex: [93366-33-7].
$C_{47}H_{39}Cl_{12}O_{11}P_3U$ M 1536.2
Green solid. Sol. CH_2Cl_2.

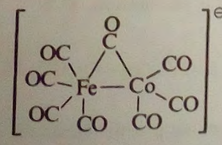
Bis-Ph_3PO complex: [88027-34-3].
$C_{44}H_{30}Cl_{12}O_{10}P_2U$ M 1444.1
Green solid. Sol. CH_2Cl_2, $CHCl_3$.

Inorg. Synth., 1967, **9**, 41 (*synth*)
Bagnall, K.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1109; 1983, 1153 (*synth, complexes, ir*)
Ivanov, A.V. *et al*, *Radiokhimiya*, 1977, **19**, 200 (*synth, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 55, *Suppl.*, 1983, C13, 151 (*rev*)
Ahmed, I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 1527 (*complexes, ir*)

$C_8CoFeO_8^{\ominus}$ IC-005870

μ-Carbonyltetracarbonyl(tricarbonylcobalt)ferrate(1−), 9CI

Octacarbonylcobaltateferrate(1−)



M 338.8 (ion)
Initially assigned di-μ-carbonyl struct. (8CI).

Bis(*triphenylphosphine*)*iminium salt:* [53217-89-3].
Rel. air-stable red cryst. (Et_2O/pentane). Sol. Et_2O, THF, $MeNO_2$. Mp 100-102° (rapid heating). With slow heating dec. without melting at 75-80°. Ir ν_{CO} 2056w, 1989m, 1953s, 1895w, 1776m (nujol).

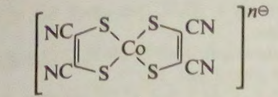
Ruff, J.K., *Inorg. Chem.*, 1968, **7**, 1818 (*synth, ir*)
Chin, H.B. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 5285 (*cryst struct*)
Horwitz, C.P. *et al*, *Organometallics*, 1985, **4**, 1117 (*synth*)

$C_8CoN_4S_4^{\ominus}$ IC-005871

Bis(maleonitriledithiolato)cobaltate(1−)

Bis[2,3-*dimercapto*-2-*butenedinitrilato*(2−)-S,S′] *Bis*[1,2-*dicyanoethenedithiolato*(2−)-S,S′]*cobaltate*(1−), *10CI*

[46760-70-7]



$n = 1$

M 339.3 (ion)

Tetrabutylammonium salt: Not isol. Sol. THF.

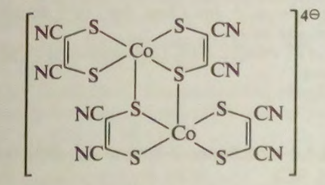
Vlček, A. *et al*, *Inorg. Chim. Acta*, 1980, **43**, 35 (*synth, kinetics*)

$C_8CoN_4S_4^{2\ominus}$ IC-005872

Bis(maleonitrilodithiolato)cobaltate(2−)

Bis[2,3-*dimercapto*-2-*butenedinitrilato*-S,S′]*cobaltate*(2−), *10CI*

[40706-01-2]



dimer

M 339.3 (ion)
Probably dimeric structure with Co—S axial interactions, as shown.

Bis-Et_4N salt: [15665-96-0].
Black solid. Dec. at 197-200°.

Bis-Ph_4P salt: [33519-88-9].
Black cryst. Sol. strongly polar solvs. Mp 247-249°.

[48164-00-7]

Inorg. Synth., 1972, **13**, 187 (*synth, props*)
Vlcek, A. *et al*, *J. Electroanal. Chem.*, 1981, **125**, 481 (*synth, electrochem*)

$C_8CoN_4S_4^{3\ominus}$ IC-005873

Bis(maleonitriledithiolato)cobaltate(3−)

Bis[2,3-*dimercapto*-2-*butenedinitrilato*(2−)-S,S′] *cobaltate*(3−), *10CI*. *Bis*[1,2-*dicyanoethenedithiolato*(2−)-S,S′]*cobaltate*(3−)

[72883-66-0]

As Bis(maleonitriledithiolato)cobaltate(1−), IC-005871 with

$n = 3$

M 339.3 (ion)
Prep. in soln. Not isol.

Vlček, A. *et al*, *Inorg. Chim. Acta*, 1980, **41**, 123 (*synth, electrochem*)

$C_8Co_2HgO_8$ IC-005874

Octacarbonyl(mercury)dicobalt, 9CI

[13964-88-0]

$(OC)_4Co—Hg—Co(CO)_4$

M 542.5
Catalyst for cyclotrimerisation of alkynes and perfluoroalkynes, intermed. in $Co_2(CO)_8$-catalysed synthesis of ketones from diarylmercury compds.
Orange cryst. (Me_2CO). Mp 81-82°. Ir ν_{CO} 2072, 2021, 2007 cm^{-1} (heptane).

Hubel, W. *et al*, *Chem. Ber.*, 1960, **93**, 103.
Lucken, E.A. *et al*, *J. Chem. Soc. A*, 1967, 148 (*nmr*)
Sheldrick, G.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1967, 1015 (*cryst struct*)
Manning, A.R., *J. Chem. Soc. A*, 1968, 1018 (*synth, ir*)
Seyferth, D. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 6192 (*use*)
Gastinger, R.C. *et al*, *J. Org. Chem.*, 1978, **43**, 159.

$C_8Co_2N_8^{8\ominus}$ IC-005875

Octakis(cyano-*C*)dicobaltate(8−), 8CI

[23705-25-1]

$[(NC)_4CoCo(CN)_4]^{8\ominus}$

M 326.0 (ion)
Bi-trigonal bipyramidal struct. with axial Co.

Octa-K salt: Bright yellow hygroscopic light-sensitive solid.

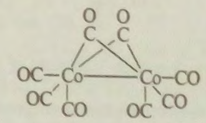
Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1954, **276**, 12 (*synth*)
Griffith, W.P. *et al*, *J. Chem. Soc. A*, 1969, 834 (*ir, raman*)

$C_8Co_2O_8$ IC-005876

Di-μ-carbonylhexacarbonyldicobalt, 10CI, 9CI

Octacarbonyldicobalt. Cobalt carbonyl ($Co_2(CO)_8$). *Dicobalt octacarbonyl*

[10210-68-1]



M 341.9
In soln. a nonbridged form exists in equilib. with the bridged form shown. Important hydroformylation catalyst. Also catalyses Fischer-Tropsch hydrogenation of CO, water gas shift reaction and the carboalkoxylation of alkyl halides and other compds. Air-sensitive orange-red cryst. Insol. H_2O; sol. org. solvs. Mp 51-52°.

▷ Highly toxic. GG0300000.

Inorg. Synth., 1946, **2**, 238; 1957, **5**, 190 (*synth*)
Adkins, H. *et al*, *J. Am. Chem. Soc.*, 1948, **71**, 3051 (*synth*)
Wender, I. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 4375 (*synth*)
Adkins, H. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 3951 (*ir, uv*)
Noack, K., *Helv. Chim. Acta*, 1964, **47**, 1555 (*ir*)
Christahl, M. *et al*, *Z. Naturforsch., B*, 1977, **32**, 637 (*uv*)
Hagen, A.P. *et al*, *Inorg. Chem.*, 1978, **17**, 1369 (*synth*)
Evans, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 626 (*cmr*)
Murai, S. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1979, **18**, 837 (*use, rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1982, **10**, 129; **11**, 162.
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 938.

C_8Cs IC-005877

Caesium graphite (CsC_8), 9CI

Caesium compd. with graphite (*1:8*), *10CI*. *Caesium-graphite intercalate*. *Caesium-graphite lamellar compd.*

[12079-66-2]

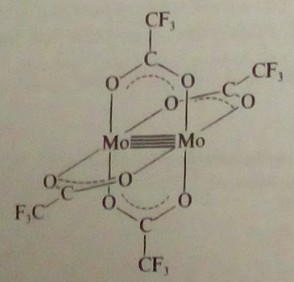
C_8Cs

M 228.9
Hexagonal. Member of a family of compds. with differing stoichiometries (C_8Cs, $C_{12}Cs$, $C_{24}Cs$ etc.). Synth. by reaction of graphite with Cs vapour. Moisture-sensitive shiny black powder. Becomes superconducting at low temps. ΔH_f° −100.4 kJ mol^{-1}; ΔG_f° −40.8 kJ mol^{-1}.
▷ Reacts violently with H_2O to form graphite and CsOH.

Lagrange, P. *et al*, *Proc. London Int. Carbon, Graphite Conf., 5th*, 1978, **2**, 660; *CA*, 1980, **92**, 224646 (*struct*)
Solin, S.A. *et al*, *J. Raman Spectrosc.*, 1981, **10**, 129 (*raman*)
Estrade-Szwarckopf, H. *et al*, *Springer Ser. Solid State Sci.*, 1981, **38**, 274; *CA*, 1982, **96**, 209617 (*Cs-133 nmr*)
Dominguez, D.D. *et al*, *Mater. Res. Soc. Symp. Proc.*, 1983, **20**, 363; *CA*, **98**, 208958 (*cmr*)

$C_8F_{12}Mo_2O_8$ IC-005878

Tetrakis[μ-(trifluoroacetato-*O*:*O*′)]dimolybdenum(*II*), 9CI
Tetrakis(trifluoroacetato)dimolybdenum(II). *Molybdenum*(II) *trifluoroacetate dimer*
[36608-07-8]

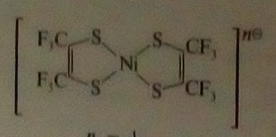


M 643.9
Mo—Mo 209 pm. Synth. by treatment of $Mo_2(OAc)_4$ with mixture of $CF_3COOH/(CF_3CO)_2O$ [10:1]. Catalyst precurser for disproportionation of propene. Mod. air-stable yellow cryst. (by subl.). Sol. Et_2O, Me_2CO, EtOH, MeOH. Subl. 180° (under 1 atm. N_2).

Cotton, F.A. *et al*, *J. Coord. Chem.*, 1971, **1**, 161 (*synth, cryst struct, ir, raman, w, ms*)
San Filippo, J. *et al*, *Inorg. Chem.*, 1973, **12**, 2326 (*raman*)
Smith, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 1742 (*use, catalyst*)
Baxendale, J.H. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 637 (*redox reaction studies*)
Cowman, C.D. *et al*, *Isr. J. Chem.*, 1977, **15**, 308 (*mcd*)
Garner, C.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1279 (*gas phase ed*)
Barry, M. *et al*, *Chem. Phys. Lett.*, 1980, **70**, 350 (*pe*)
Brown, D.I., *J. Chem. Soc., Dalton Trans.*, 1980, 1118 (*struct, bonding*)
Cotton, F.A. *et al*, *Inorg. Chim. Acta*, 1988, **144**, 109 (*use*)
Islam, M.Q. *et al*, *J. Fluorine Chem.*, 1990, **48**, 429 (*use*)

$C_8F_{12}NiS_4^{\ominus}$ IC-005879

Bis[1,2-bis(trifluoromethyl)ethane-1,2-dithiolato]nickelate(1−)
Bis(1,1,1,4,4,4-hexafluoro-2-butene-2,3-dithiolato)nickelate(1−)
[16674-52-5]



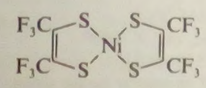
$n = 1$

M 511.0 (ion)
Square planar. Formed from Bis[1,1,1,4,4,4-hexafluoro-2-butene-2,3-dithiolato(2−)-*S*,*S*′]nickel, IC-005880 + planar organic molecules giving stacked structure with one dimensional electrical conductance. Interesting magnetic properties. Ligand formerly known as thiete.
Phenothiazine salt: [53142-51-1].
$C_{20}H_9F_{12}NNiS_5$ M 710.2
Dark brown cryst. (C_6H_6/pentane). Sol. C_6H_6, CH_2Cl_2. Ferrimagnetic.
Tetrathiafulvalene salt: [54992-69-7]. *2-(1,3-dithiol-2-ylidene)-1,3-dithiol salt, 9CI*
Black needles (C_6H_6). Sol. C_6H_6, MeCN. Formulated as ionic struct. on basis of magnetic props. $\mu_{eff} = 1.7\mu_B$; departs from Curie-Weiss behaviour <35K.
[34257-49-3]

Davison, A. *et al*, *Inorg. Chem.*, 1963, **2**, 1227 (*synth, esr, magnetism, polarography*)
Wing, R.M. *et al*, *Inorg. Chem.*, 1970, **9**, 471 (*synth, cryst struct, magnetism*)
Geiger, W.E. *et al*, *J. Phys. Chem.*, 1971, **75**, 2387 (*synth, uv-vis, esr, magnetism, phenothazine salt*)
Jacobs, I.S. *et al*, *AIP Conf. Proc.*, 1974, **24**, 355; *CA*, 1975, **83**, 141003 (*magnetism*)
Singhabhandhu, A. *et al*, *Inorg. Chem.*, 1975, **14**, 318 (*cryst struct, phenothiazine salt*)
Interrante, L.V. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 889 (*synth, esr, magnetism, elec cond*)
Jacobs, I.S. *et al*, *Physica B+C (Amsterdam)*, 1977, **86-88**, 655 (*magnetism*)

$C_8F_{12}NiS_4$ IC-005880

Bis[1,1,1,4,4,4-hexafluoro-2-butene-2,3-dithiolato(2−)-*S*,*S*′]nickel, 9CI
Bis[1,2-bis(trifluoromethyl)ethene-1,2-dithiolato]nickel.
Bis[1,2-bis(trifluoromethyl)-1,2-ethylenedithiolato]nickel.
Bis(hexafluoro-2,3-butanedithione)nickel
[18820-78-5]



M 511.0
Air stable black cryst. (C_6H_6). Mp 134-135°.
Perylene complex: [25168-79-0].
Cryst.
[14057-77-3, 15349-12-9, 17410-46-7, 55401-06-4]

Inorg. Synth., 1967, **10**, 8 (*synth, props, derivs*)
Schmitt, R.D. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 4394 (*cryst struct, deriv*)
Schläpfer, C.W. *et al*, *Inorg. Chem.*, 1975, **14**, 1338 (*ir*)

$C_8F_{12}O_8Pb$ IC-005881

Tetrakis(trifluoroacetato-*O*)lead
Lead tetratrifluoroacetate

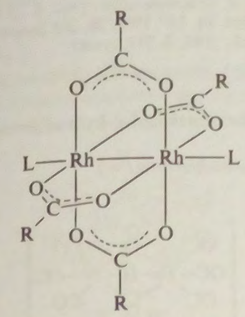
$(F_3CCOO)_4Pb$

M 659.2
Reagent for plumbylation of aromatic compds. Prepd. *in situ* from $Pb(OAc)_4$ and CF_3COOH.

De Vos, D. *et al*, *Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1973, **92**, 701; 1974, **94**, 97.

$C_8F_{12}O_8Rh_2$ IC-005882

Tetrakis[μ-(trifluoroacetato-*O*:*O*′)]dirhodium(*II*)
[31126-95-1]



L = donor molecule
R = CF_3

M 657.8
Forms a variety of adducts with two donor ligands. Anhydrous compd. obt. by heating dihydrate at 150° for 30 mins. Blue-green cryst. at r.t., green at high temp., purple at 77K. Rapidly absorbs H_2O. Sol. H_2O, THF, EtOH, Me_2CO, MeCN. Subl. 350°.
Dihydrate: [70084-34-3]. *Diaquatetrakis[μ-(trifluoroacetato-O:O′)]dirhodium*(II). *Rhodium*(II) *acetate hydrate*
$C_8H_4F_{12}O_{10}Rh_2$ M 693.9
Dark green cryst.
Bis-EtOH complex: [15259-45-7].
$C_{12}H_{12}F_{12}O_{10}Rh_2$ M 750.0
Cryst., loses EtOH over several days in air. Sol. $CHCl_3$.
Bis-DMSO complex: [72665-42-0]. *Bis(dimethyl sulfoxide) tetrakis(trifluoroacetato)dirhodium*(II).
Bis[sulfinylbis[methane]-O]tetrakis[μ-(trifluoroacetato-O:O′)]dirhodium(II), *10CI*. *Rhodium*(II) *trifluoroacetate DMSO complex*
$C_{12}H_{12}F_{12}O_{10}Rh_2S_2$ M 814.1
Dark blue cryst. ($CHCl_3/C_6H_6$). Dichroic: red in some orientations, in transmitted light. DMSO ligands coordinate through O.
Bis-dimethylsulfone complex: [77590-01-3]. *Bis(dimethyl sulfone)tetrakis(trifluoroacetato)dirhodium*(II).
Bis[sulfonylbis[methane]-O]tetrakis[μ-(trifluoroacetato-O:O′)]dirhodium(II), *10CI*. *Rhodium*(II) *trifluoroacetate dimethylsulfone complex*
$C_{12}H_{12}F_{12}O_{12}Rh_2S_2$ M 846.1
Dark green cryst. or blue-green powder.
Monomer: Rhodium(II) *trifluoroacetate*. *Rhodium bis-trifluoroacetate*
$C_4F_6O_4Rh$ M 328.9
Not separately identified.

Johnson, S.A. *et al*, *Inorg. Chem.*, 1963, **2**, 961 (*synth*)
Kitchens, J. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 2415.
Kitchens, J. *et al*, *Thermochim. Acta*, 1970, **1**, 537 (*props*)
Porai-Koshits, M.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 716 (*synth, cryst struct, bis-EtOH complex*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1980, **19**, 2347; 1981, **20**, 2703; 1982, **21**, 2667 (*synth, ir, cryst struct, complexes*)

$C_8F_{12}O_8Th$ IC-005883

Thorium(*IV*) trifluoroacetate
Tetrakis(trifluoroacetato-O,O′)thorium
[16424-71-8]

$Th(OCOCF_3)_4$

M 684.1
White cryst. Affords CO, CO_2, COF_2, CF_3COF, $(CF_3CO)_2O$ on dec. Forms complexes with wide range of Lewis bases at 272°.
Monohydrate:
$C_8H_2F_{12}O_9Th$ M 702.1
White cryst. Dec. to ThF_4 >310°.
Tetrakis-(N,N′-dimethylurea) complex: [93366-22-4].
$C_{20}H_{32}F_{12}N_8O_{12}Th$ M 1036.5
White solid. Sol. CH_2Cl_2.
Bis-tetramethylurea complex: [93393-33-0].
$C_{18}H_{24}F_{12}N_4O_{10}Th$ M 916.4
White solid. Sol. CH_2Cl_2.
Tris-(N,N-dimethylacetamide) complex: [60447-58-7].
$C_{20}H_{27}F_{12}N_3O_{11}Th$ M 945.4
Colourless cryst. Sol. $CHCl_3$.
Tetrakis-DMSO complex: [88027-35-4].
$C_{16}H_{24}F_{12}O_{12}S_4Th$ M 996.6
White solid. Sol. CH_2Cl_2.
Bis-Ph_2SO complex: [88006-23-9].
$C_{32}H_{20}F_{12}O_{10}S_2Th$ M 1088.6
White solid. Sol. CH_2Cl_2, $CHCl_3$.
Tris-Me_3PO complex: [88006-09-1].
$C_{17}H_{27}F_{12}O_{11}P_3Th$ M 960.3
White solid. Sol. CH_2Cl_2.
Tris-Me_2PhPO complex: [93366-26-8].
$C_{32}H_{33}F_{12}O_{11}P_3Th$ M 1146.5
White solid. Sol. CH_2Cl_2.
Tris-Ph_2MePO complex: [93366-30-4].
$C_{47}H_{39}F_{12}O_{11}P_3Th$ M 1332.7
White solid. Sol. CH_2Cl_2.
Bis-Ph_3PO complex: [88006-14-8].
$C_{44}H_{30}F_{12}O_{10}P_2Th$ M 1240.6
White solid. Sol. CH_2Cl_2.

Hara, R. *et al*, *J. Am. Chem. Soc.*, 1954, **76**, 4285 (*synth*)
Sarton, P. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1964, **3**, 376 (*synth*)
Bagnall, K.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1109; 1983, 1153 (*complexes, synth, ir*)
Ahmed, I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 1527 (*complexes, ir*)
Matseev, Yu.S. *et al*, *Koord. Khim.*, 1985, **11**, 207 (*synth, ir, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. **44**, *Suppl.*, 1988, 55; *Suppl.*, 1985, **E**, 49 (*rev*)

$C_8F_{12}O_8U$ IC-005884

Uranium(*IV*) trifluoroacetate
Tetrakis(trifluoroacetato)uranium
[7638-38-2]

$U(OCOCF_3)_4$

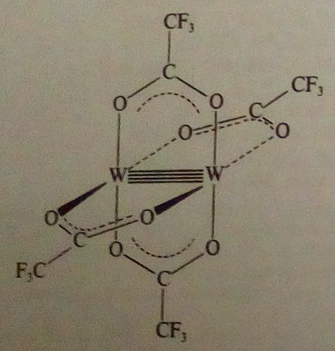
M 690.0
Light green solid. Sl. sol. C_6H_6, F_3CCOOH. Forms complexes with wide range of Lewis bases.
Tris(N,N′-dimethylurea) complex: [93366-23-5].
$C_{17}H_{24}F_{12}N_6O_{11}U$ M 954.4
Green solid. Sol. CH_2Cl_2.
Bis-tetramethylurea complex: [93393-34-1].
$C_{18}H_{24}F_{12}N_4O_{10}U$ M 922.4
Green solid. Sol. CH_2Cl_2.
Tetrakis-DMSO complex: [88006-18-2].
$C_{16}H_{24}F_{12}O_{12}S_4U$ M 1002.6
Green solid. Sol. CH_2Cl_2.
Bis-Ph_2SO complex: [88006-24-0].
$C_{32}H_{20}F_{12}O_{10}S_2U$ M 1094.6
Green solid. Sol. CH_2Cl_2, $CHCl_3$.
Tetrakis-Me_3PO complex: [88006-10-4].
$C_{20}H_{36}F_{12}O_{12}P_4U$ M 1058.4
Green solid. Sol. CH_2Cl_2, $CHCl_3$.
Tris-Me_2PhPO complex: [93366-27-9].

$C_{32}H_{33}F_{12}O_{11}P_3U$ M 1152.5
Green solid. Sol. CH_2Cl_2, THF.
Tris-$MePh_2PO$ complex: [93366-31-5].
$C_{47}H_{39}F_{12}O_{11}P_3U$ M 1338.7
Green solid. Sol. CH_2Cl_2.
Tris-Ph_3PO complex: [88006-15-9].
$C_{62}H_{45}F_{12}O_{11}P_3U$ M 1524.9
Green solid. Sol. CH_2Cl_2, $CHCl_3$.
Bis-[2.2.2]cryptand complex: Green cryst. + H_2O. Sol. MeCN. Four U atoms are linked by bridging trifluoroacetates and waters to form a neutral tetramer. Cryptands are not coordinated. Bicapped trigonal prismatic at U.

Selbin, J. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1385 (*synth, ir*)
Bagnall, K.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1109, 1111; 1983, 1153 (*complexes, synth, ir*)
Devillardi, G.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 90 (*synth, adducts, struct*)
Gill, M.S. *et al*, *Indian J. Chem., Sect. A*, 1986, **25**, 687 (*synth*)
Charpin, P. *et al*, *Acta Crystallogr., Sect. C*, 1990, **46**, 1778 (*adduct, cryst struct*)

$C_8F_{12}O_8W_2$ IC-005885

Tetrakis[μ-(trifluoroacetato-*O*:*O'*)]ditungsten(*II*), 10CI
[77479-85-7]

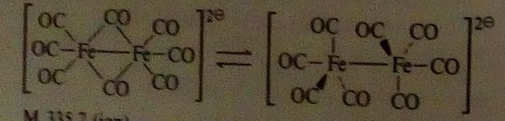


M 819.7
First quadruply-bonded W(*II*) carboxylate. Bright-yellow air-sensitive cryst. $Subl_{0.0001}$ 100-130°. Dec. at *ca.* 200°.

Cotton, F.A. *et al*, *Inorg. Chem.*, 1981, **20**, 3880.
Santure, D.J. *et al*, *Inorg. Chem.*, 1983, **22**, 1877; 1984, **23**, 938 (*synth, props*)

$C_8Fe_2O_8^{2\ominus}$ IC-005886

Octacarbonyldiferrate(2−), 9CI, 8CI
Di-μ-carbonylhexacarbonyldiferrate(2−)
[25463-33-6]

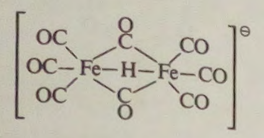


M 335.7 (ion)
May have bridged-nonbridged equilib. Ir ν_{CO} 1910m, 1860s, 1835w cm^{-1}.
Di-Na salt: [64913-30-0].
Synth. from $Fe(CO)_5$ and $Na(C_{10}H_8)$ in THF. Bright yellow solid when dry; addition of THF causes colour change to orange.
▷ Dry salt is pyrophoric.
Bis-Et_4N salt: [26024-88-4].
V. air-sensitive brick-red cryst. Insol. most org. solvs.; spar. sol. THF; sol. DMF.

Farmery, K. *et al*, *J. Chem. Soc. A*, 1969, 2339 (*synth, ir, mössbauer*)
Chin, H.B. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 5285.
Onaka, S. *et al*, *Inorg. Chem.*, 1976, **15**, 915 (*raman, struct*)
Sumner, C.E. *et al*, *Organometallics*, 1982, **1**, 1350.
Inorg. Synth., 1986, **24**, 157; 1990, **28**, 203 (*synth*)
Organomet. Synth., 1986, **3**, 217 (*synth*)

$C_8HFe_2O_8^{\ominus}$ IC-005887

Di-μ-carbonylhexacarbonyl-μ-hydrodiferrate(1−), 9CI, 8CI
Octacarbonylhydrodiferrate(1−)
[20960-30-9]

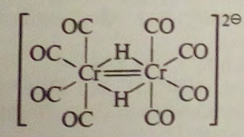


M 336.7 (ion)
Reducing agent, e.g. for conversion of enamines to amines.
Na salt: [60308-01-2].
Reddish-brown in soln.
Et_4N salt: [26062-33-9].
V. air-sensitive mustard-yellow solid. Sometimes pyrophoric.

Farmery, K. *et al*, *J. Chem. Soc. A*, 1967, 2339 (*synth, mössbauer*)
Mitsudo, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 1506 (*use*)
Onaka, S. *et al*, *Inorg. Chem.*, 1976, **15**, 915 (*raman*)
Collman, J.P. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 4685 (*synth, ir, pmr, cryst struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 340 (*synth, use*)
Sumner, C.E. *et al*, *Organometallics*, 1982, **1**, 1350 (*synth*)

$C_8H_2Cr_2O_8^{2\ominus}$ IC-005888

Octacarbonyl-μ-dihydrodichromate(2−)

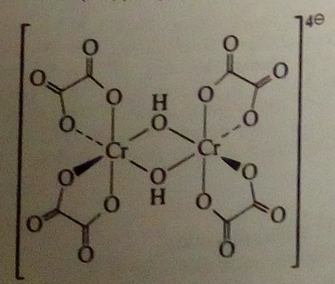


M 330.0 (ion)
Bis-Et_4N salt: [84850-72-6].
Air-sensitive burgundy cryst.

Ellis, J.E. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 2296 (*synth*)

$C_8H_2Cr_2O_{18}^{4\ominus}$ IC-005889

Di-μ-hydroxytetrakis(oxalato)dichromate(4−)
Di-μ-hydroxobis[bis(oxalato)chromate(III)].
Tetrakis[ethanedioato(2−)-O,O']di-μ-hydroxydichromate(III)(4−),*10CI*



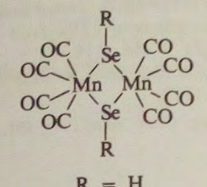
M 490.0 (ion)
Roughly octahedral geometry about each Cr.

Tetra-Na salt: [63121-47-1].
Cryst. + $6H_2O$ (H_2O).

Scaringe, R.P. *et al*, *Inorg. Chim. Acta*, 1977, **22**, 175 (*cryst struct, synth, magnetism*)

$C_8H_2Mn_2O_8Se_2$ IC-005890

Octacarbonyldi-μ-selenyldimanganese, 10CI
Di-μ-hydroselenobis(tetracarbonylmanganese)
[62364-60-7]

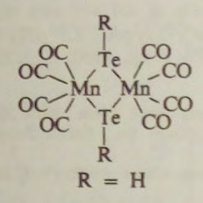


M 493.8
Synth. from $MnBr(CO)_5$ and $Se(SnMe_3)_2$ followed by HCl. Yellow-brown cryst. Ir ν_{CO} 2064, 2005, 1997, 1974 cm^{-1} (cyclohexane). Dec. at 180°.

Küllmer, V. *et al*, *Chem. Ber.*, 1977, **110**, 228 (*synth, ir, pmr*)

$C_8H_2Mn_2O_8Te_2$ IC-005891

Octacarbonyldi-μ-telluryldimanganese, 10CI
Di-μ-(hydrotelluro)bis(tetracarbonylmanganese)
[62364-61-8]

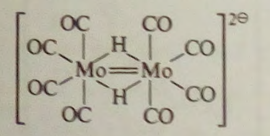


M 591.1
Synth. from $MnBr(CO)_5$, $Te(SnMe_3)_2$ followed HCl. Light-brown cryst. Ir ν_{CO} 2054, 2000, 1998, 1974, 1964 cm^{-1} (cyclohexane); dec. at 70°.

Küllmer, V. *et al*, *Chem. Ber.*, 1977, **110**, 228 (*synth, ir, pmr*)

$C_8H_2Mo_2O_8^{2\ominus}$ IC-005892

Octacarbonyl-μ-dihydrodimolybdate(2−)

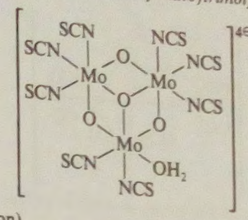


M 417.9 (ion)
Bis-Et_4N salt: [84850-68-0].
Orange air-sensitive cryst.

Ellis, J.E. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 2296 (*synth*)

$C_8H_2Mo_3N_8O_5S_8^{4\ominus}$ IC-005893

Aqua-μ_3-oxotri-μ-oxooctakis(thiocyanato-*N*)trimolybdate(*IV*)(4−), 11CI
Aqua-μ_3-oxotri-μ-oxoocta(thiocyanato)trimolybdate(IV)



M 834.5 (ion)
Tetrakis-Me_4N salt: [82428-66-8].
Tan-green cryst. (aq. MeCN).

Schlemper, E.O. *et al*, *Cryst. Struct. Commun.*, 1982, **11**, 89 (*cryst struct, synth*)

$C_8H_2O_8Os_2$ IC-005894

Octacarbonyldihydrodiosmium, 8CI
[25685-05-6]

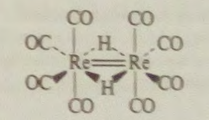
$(OC)_4OsH—OsH(CO)_4$

M 606.4
Colourless oil. $Bp_{0.01}$ 40°.

Moss, J.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1969, 800.
Moss, J.R. *et al*, *Inorg. Chem.*, 1977, **16**, 75 (*synth, ir, pmr, ms*)

$C_8H_2O_8Re_2$ IC-005895

Octacarbonyldi-μ-hydrodirhenium, 10CI
[38887-05-7]

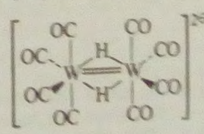


M 598.5
Synth. from $Ph_2SiH_2Re_2(CO)_8$ and H_2SiO_3. Yellow cryst. (CH_2Cl_2/*n*-hexane at −20°); mod. air-stable, dec. slowly in light. Ir ν_{CO} 2093, 2020, 2000, 1979 cm^{-1} (cyclohexane).

Bennett, M.J. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 6232 (*synth, ir, pmr, cryst struct, ms, raman*)
Andrews, M.A. *et al*, *Inorg. Chem.*, 1977, **16**, 1556 (*synth, ms*)
Epstein, R.A. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 3847 (*synth, ir, ue*)

$C_8H_2O_8W_2^{2\ominus}$ IC-005896

Octacarbonyldi-μ-hydroditungstate(2−), 9CI



M 593.7 (ion)
Bis-Et_4N salt: Red cryst.

Davison, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 691 (*synth*)
Churchill, M.R. *et al*, *Inorg. Chem.*, 1974, **13**, 2413 (*cryst struct*)

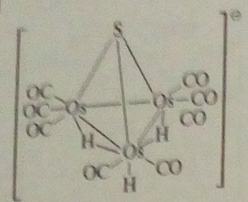
IC-005897

$C_8H_3O_8Os_3S^{\ominus}$

Octacarbonyldi-μ-hydrohydro-μ_3-thioxotriosmate(1−)

Octacarbonyldihydro-μ_3-thioxotriosmate(1−)

[74325-98-7]



M 829.7 (ion)

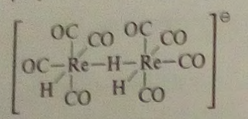
No phys. props. reported.

Johnson, B.F.G. *et al*, *J. Organomet. Chem.*, 1980, **190**, C91 (*synth, pmr*)

IC-005898

$C_8H_3O_8Re_2^{\ominus}$

Octacarbonyl-μ-hydrodihydrodirhenate(1−)



M 599.5 (ion)

Et_4N salt: [107890-38-0].

Cream solid (THF/heptane). Ir ν_{CO} 2080vw, 2054mw, 1973vs, 1953sh, 1916ms cm^{-1} (THF).

Beringhelli, T. *et al*, *Organometallics*, 1987, **6**, 1365 (*synth, struct, ir, pmr, cmr*)

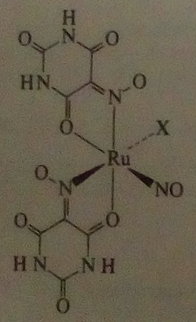
IC-005899

$C_8H_4BrN_7O_9Ru$

Bromo(nitrosyl)bis(violurato)ruthenium

Bromo(nitrosyl)bis(2,4,5,6(1H,3H)-pyrimidinetetrone-5-oximate-N^5,O^4)ruthenium, 9CI. Bis(alloxan-5-oximato)bromo(nitrosyl)ruthenium

[57546-18-6]



X = Br

M 523.1

Prepd. by treating the Na salt of Tris(violurato)ruthenate(*II*)(1−), IC-007425 with $NaNO_2$ in aq. HBr. Orange solid. Ir ν_{NO} 1949, 1940; ν_{RuBr} 240 cm^{-1}.

[67529-74-2]

Sueur, S. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1975, **281**, 401 (*synth*)

Bremard, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2307 (*synth, ir, uv*)

Bremard, C. *et al*, *Inorg. Chem.*, 1978, **17**, 3220 (*kinetics*)

IC-005900

$C_8H_4Br_8O_8Zr$

Tetrakis(dibromoacetato-*O*,*O*′)zirconium(*IV*), 11Cl

[97894-98-9]

$Zr(OOCCHBr_2)_4$

M 958.5

8-Coordinate. Synth. by refluxing $ZrCl_4$ in dibromoacetic acid. White solid. Sol. MeCN, $PhNO_2$, DMF. Insol. C_6H_6. Mp >270°.

Bis-Py complex: [97894-88-7]. *Tetrakis(dibromoacetato-O,O′)bis(pyridine)zirconium*(IV), *11Cl*

$C_{18}H_{14}Br_8N_2O_8Zr$ M 1116.7

Light yellow solid. Sol. MeCN, $PhNO_2$, DMF; insol. C_6H_6. Mp 109-111°.

Puri, J.K. *et al*, *Inorg. Chim. Acta*, 1985, **101**, 135 (*synth, ir, pmr, cmr, deriv*)

IC-005901

$C_8H_4ClN_7O_9Ru$

Chloro(nitrosyl)bis(violurato)ruthenium

Chloro(nitrosyl)bis(2,4,5,6(1H,3H)-pyrimidinetetrone 5-oximato-N^5,O^4)ruthenium, 9Cl

[57409-08-2]

As Bromo(nitrosyl)bis(violurato)ruthenium, IC-005899 with

X = Cl

M 478.6

Prepd. by treating the Na salt of Tris(violurato) ruthenate(*II*)(1−), IC-007425 with $NaNO_2$ in HCl. Yellow solid. pK_{a1} 2.3; pK_{a2} 3.5; pK_{a3} 8.9; pK_{a4} 10.2 (0.5*M* NaCl, 25°). Ir ν_{NO} 1950; ν_{RuCl} 320 cm^{-1}.

[67529-73-1]

Sueur, S. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 2037 (*pK*)

Bremard, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2307 (*synth, ir, uv*)

Brenard, C. *et al*, *Inorg. Chem.*, 1978, **17**, 3220; 1979, **18**, 1549 (*synth, reactions*)

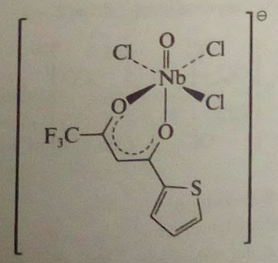
Kuek, H.T. *et al*, *Inorg. Chim. Acta*, 1981, **52**, 1 (*synth*)

IC-005902

$C_8H_4Cl_3F_3NbO_3S^{\ominus}$

Trichlorooxo[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedionato-*O*,*O*′]niobate(*V*)(1−), 10Cl

Oxotrichloro(1,1,1-trifluoro-4-thenoyl-2,4-butanedionato) niobate(V)(*1*−)



M 436.4 (ion)

Distorted octahedral, Nb is approx. 30 pm above the Cl_3O plane, towards the oxo group.

Et_4N salt: [55188-99-3].

Synth. from $Et_4N[NbOCl_4]$ + the ligand in MeCN.

[70332-74-0]

Kergoat, R. *et al*, *J. Less-Common Met.*, 1975, **39**, 91 (*synth*)

Daran, J.C. *et al*, *Inorg. Chim. Acta*, 1979, **33**, 81 (*cryst struct*)

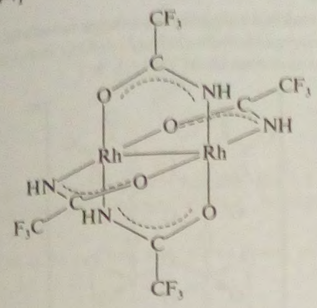
Calves, J.Y. *et al*, *Inorg. Chim. Acta*, 1979, **33**, 95 (*reactions*)

IC-005903

$C_8H_4F_{12}N_4O_4Rh_2$

Tetrakis[μ-(2,2,2-trifluoroacetamido-*N*:*O*)]dirhodium(*II*), 11Cl

[81988-04-7]



M 653.9

Sol. Me_2CO, MeOH.

Bis-Py complex: [82464-58-2]. *Bis(pyridine)tetrakis[μ-(2,2,2-trifluoroacetamido-N:O)]dirhodium*(II), *11Cl*

$C_{18}H_{14}F_{12}N_6O_4Rh_2$ M 812.1

Yellow cryst. Py bound to Rh—Rh nucleus in axial positions.

Dennis, A.M. *et al*, *Inorg. Chem.*, 1983, **22**, 1522 (*synth, uv, pmr, F-19 nmr, cryst struct, deriv*)

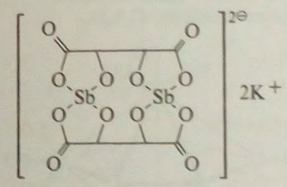
IC-005904

$C_8H_4K_2O_{12}Sb_2$

Antimony potassium tartrate, USAN

Dipotassium bis[μ-[tartrato(4−)]]diantimonate(2−). Tartar emetic

[28300-74-5]



M 613.8

Antischistosomal, emetic, expectorant. $[\alpha]_D^{20}$ +140.69° (c, 2 in H_2O).

▷CC6825000.

[11071-15-1]

Rosario, S., *Boll. Soc. Ital. Biol. Sper.*, 1928, **3**, 287; *CA*, **22**, 3231 (*pharmacol*)

Volmar, Y. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci.*, 1938, **206**, 1904 (*synth*)

U.S. Pat., 2 391 297, (1945); *CA*, **40**, 1284 (*synth*)

Ercoli, N., *Proc. Soc. Exp. Biol. Med.*, 1968, **129**, 284 (*metab*)

Gress, M.E. *et al*, *Inorg. Chim. Acta*, 1974, **8**, 209 (*cryst struct*)

Salem, F.S. *et al*, *J. Drug Res.*, 1980, **12**, 43 (*pharmacol*)

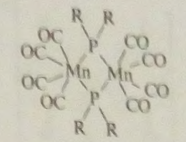
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 756.

IC-005905

$C_8H_4Mn_2O_8P_2$

Octacarbonyldi-μ-phosphinodimanganese

[87067-72-9]



R = H

M 399.9

Air-stable yellow needles or plates (CH_2Cl_2). Mp 182° Subl.$_{0.01}$ 65°. Ir ν_{CO} 2060s, 1998vs, 1978s, 1945w cm^{-1} (cyclopentane).

Schäfer, H. *et al*, *Z. Anorg. Allg. Chem.*, 1983, **501**, 111; 1985, **529**, 157 (*pmr, synth, P-31 nmr, ir, ms*)

Deppisch, B. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **519**, 53 (*struct*)

IC-005906

$C_8H_4N_8O_{11}Ru$

Nitro(nitrosyl)bis(violurato)ruthenium

(Nitrito-N)nitrosylbis(2,4,5,6(1H,3H)-pyrimidinetetrone 5-oximato-N^5,O^4)ruthenium, 9Cl. Nitro(nitrosyl) bis(2,4,5,6(1H,3H)-pyrimidinetetrone 5-oximato)ruthenium

[67505-83-3]

As Bromo(nitrosyl)bis(violurato)ruthenium, IC-005899 with

$X = NO_2$

M 489.2

cis-Octahedral. Prepd. by treating Na salt of Tris(violurato)ruthenate(*II*)(1−), IC-007425 with $NaNO_2$ in $HClO_4$. Yellow solid. Ir ν_{NO} 1956 cm^{-1}.

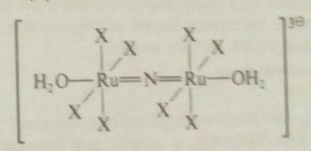
Bremard, C. *et al*, *Inorg. Chem.*, 1978, **17**, 3220 (*synth, ir, uv*)

IC-005907

$C_8H_4N_9O_2Ru_2S_8^{3\ominus}$

Diaqua-μ-nitridooctakis(thiocyanato-*N*)diruthenate(3−), 9Cl

μ-Nitridobis[aquatetrakis(thiocyanato)ruthenate(IV)]



X = NCS

M 716.8 (ion)

Tri-K salt: [27119-65-9].

$C_8H_4K_3N_9O_2Ru_2S_8$ M 834.1

Prepd. by treating $[Ru_2NCl_5(OH_2)_2]^{3\ominus}$ with K[SCN]. Brown salt; diamagnetic. Ir ν_{Ru_2N} 1037 cm^{-1}.

Cleare, M.J. *et al*, *J. Chem. Soc. A*, 1970, 1117 (*synth, ir*)

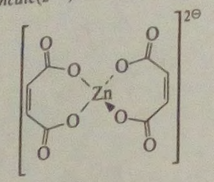
Good, M.L. *et al*, *J. Phys. Chem.*, 1984, **88**, 483.

IC-005908

$C_8H_4O_8Zn^{2\ominus}$

Bis[2-butenedioato(2−)-*O,O′*]zincate(2−)

Bis(maleato)zincate(2−)



M 293.5 (ion)

Di-H compd.: [38883-82-8].
$C_8H_6O_8Zn$ M 295.5
Cryst. + $4H_2O$ (H_2O).

Saroja, K. *et al*, *Curr. Sci.*, 1972, **41**, 599 (*synth, struct*)

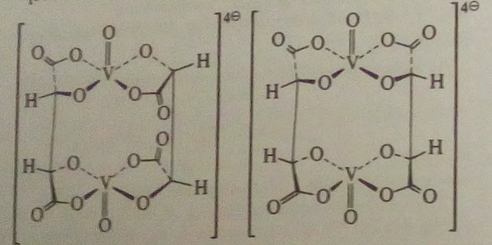
IC-005909

$C_8H_4O_{14}V_2^{4\ominus}$

Dioxobis[μ-tartrato(4−)]divanadate(*IV*)(4−)

Bis[μ-[2,3-dihydroxybutanedioato(4−)-$O^1,O^2:O^3,O^4$]] dioxodivanadate(IV)(4−), *11Cl*

[36470-81-2]



Bis-(2R,3R)tartrato-form (2R,3R)(2S,3S)-*tartrato-form*

M 425.9 (ion)

Various isomeric forms have been isolated as have those of the corresponding mono- and di-methyl tartrates. A number of magnetic and esr studies have been reported. The ion may be synth. in aq. soln. by reducing V_2O_5 with tartaric acid. Salts may be produced by adding the appropriate hydroxide. Brown or purple solids depending on the tartrate isomer.

Bis(2R,3R)tartrato-form

trans-*form*

Tetra-NH_4 salt: Ammonium vanadyl (+)-tartrate

Synth. from $VO(acac)_2$ + tartaric acid followed by NH_4OH aq. Inhibits cholesterol synth. in brain tumours. Purple cryst. + $2H_2O$.

(2R,3R)(2S,3S)tartrato-form

cis-form. dl-*tartrate-form*

Tetra-Na salt: [19426-38-1]. *Sodium vanadyl tartrate*

Synth. by reducing V_2O_5 with tartaric acid and adding NaOH to the resulting aq.soln. Brown cryst. + $12H_2O$.

Tetra-Et_4N salt: [75282-40-5].

Purple cryst. + $8H_2O$ (H_2O).

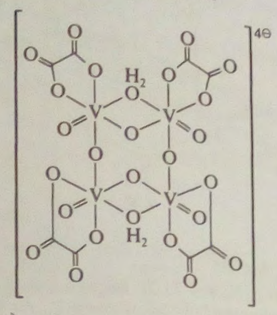
[15976-35-9, 36421-88-2, 47315-62-8, 59366-65-3]

U.S. Pat., 3 076 830, (1963); *CA*, **58**, 12375c (*synth, NH_4 salt, cholesterol inhib*)
Tapscott, R.E. *et al*, *Inorg. Chem.*, 1967, **6**, 735 (*synth, esr, magnetism, un-cit. deriv*)
Forrest, J.G. *et al*, *J. Chem. Soc. A*, 1967, 1312 (*cryst struct, NH_4 salt monohydrate*)
Tapscott, R.E. *et al*, *Inorg. Chem.*, 1968, **7**, 356 (*cryst struct, Na salt, dodecahydrate*)
Crawford, Van.H. *et al*, *J. Mol. Struct.*, 1977, **38**, 141 (*esr, magnetism, Na salt*)
Ortega, R.B. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 1786 (*cryst struct, Et_4N salt octahydrate*)
Anaya, T.M. *et al*, *Inorg. Chim. Acta*, 1981, **49**, 11 (*soln kinetics*)

$C_8H_4O_{26}V_4^{4\ominus}$ IC-005910

Diaquatetrakis(oxalato)octaoxotetravanadate(*V*)(4−)

Di-μ-aquatetrakis[ethanedioato(2−)-O,O′]tetra-μ-oxotetraoxotetravanadate(V)(4−), *9Cl*



M 719.8 (ion)

Octahedral at all V's.

Tetra-K salt: [61497-95-8].

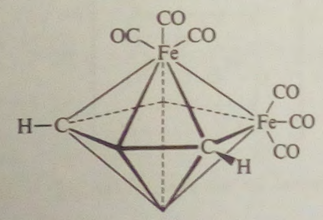
Synth. from KVO_3 and oxalic acid in aq. soln. Deep red solid + $6H_2O$.

Preuss, F. *et al*, *Chem. Ber.*, 1969, **102**, 3046 (*synth, ir*)
Drew, R.E. *et al*, *Can. J. Chem.*, 1974, **52**, 2184 (*synth*)
Rieskamp, H. *et al*, *Chem. Ber.*, 1976, **109**, 2090 (*cryst struct*)

$C_8H_5B_3Fe_2O_6$ IC-005911

Hexacarbonyl[μ-[(1,4,5-η:2,3,4,5-η)-pentahydro-2,4-dicarbapentaborato(2−)]]diiron, 9CI

1,2,3,5-(Hexacarbonyldiiron)-$C_2B_3H_5$



M 341.2

Orange liq.

Miller, V.R. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 3090 (*synth, ir, pmr, nmr*)

IC-005912

$C_8H_5N_7O_{10}Ru$

Hydroxy(nitrosyl)bis(violurato)ruthenium

Hydroxy(nitrosyl)bis(2,4,5,6(1H,3H)-pyrimidinetetrone 5-oximato-N^5,O^4)ruthenium, 9CI

[67505-82-2]

As Bromo(nitrosyl)bis(violurato)ruthenium, IC-005899 with

X = OH

M 460.2

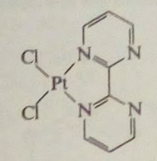
cis-Octahedral. Prepd. by heating the Na salt of Tris(violurato)ruthenate(*II*)(1−), IC-007425 with $NaNO_2$ in $HClO_4$. Yellow solid. Ir ν_{NO} 1905 cm^{-1}.

Bremard, C. *et al*, *Inorg. Chem.*, 1978, **17**, 3220 (*synth, ir, uv*)
Bremard, C. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 715 (*synth*)

$C_8H_6Cl_2N_4Pt$ IC-005913

(2,2′-Bipyrimidine-*N,N′*)dichloroplatinum(*II*), 10CI

[68976-09-0]



M 424.1

Also formed as many solvates. See also Bis(2,2′-bipyrimidine-*N,N′*)platinum(*II*)(2+), IC-009235. Orange solid.

Kiernan, P.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 1127 (*synth*)

$C_8H_6F_6O_8Rh_2$ IC-005914

Bis(acetato)bis(trifluoroacetato)dirhodium(*II*)

$Rh_2(OAc)_2(OOCCF_3)_2$

M 549.9

Prob. has dinuclear $M_2(O_2CR)_4$ struct. Synth. as an intermed. in the substitution reaction of $Rh_2(OAc)_4$ and trifluoroacetic acid.

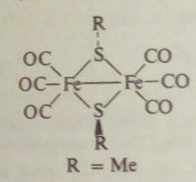
Bear, J.L. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 3479 (*synth, pmr, kinetics, ms*)

$C_8H_6Fe_2O_6S_2$ IC-005915

Hexacarbonylbis[μ-(methanethiolato)]diiron, 9CI

Di-μ-methanethiolatobis[tricarbonyliron(0)]

[14878-96-7]



trans-form

R = Me

M 373.9

Used in refining of thermal cracking of gasolines.

cis-form [19976-87-5]

syn-*form*

Air-stable orange cryst. (pentane). Sol. pentane. Mp 112-114°.

trans-form [19976-88-6]

anti-*form*

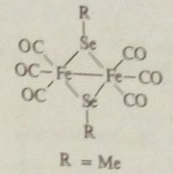
Air-stable red cryst. (pentane). Sol. pentane. Mp 70-71°. $Subl._{0.1}$ 50°.

King, R.B., *J. Am. Chem. Soc.*, 1962, **84**, 2460 (*synth, isom, ir, pmr*)
Dahl, L.F. *et al*, *Inorg. Chem.*, 1963, **2**, 328 (*struct*)
King, R.B. *et al*, *Inorg. Chem.*, 1965, **4**, 1663 (*synth, pmr*)
Lauterbur, P.C. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 3266 (*cmr*)
Organomet. Synth., 1965, **1**, 180 (*synth*)
Büttner, H. *et al*, *Inorg. Chem.*, 1972, **11**, 971 (*pmr*)
Adams, R.D. *et al*, *Inorg. Chem.*, 1975, **14**, 1395 (*pmr, cmr*)
Le Borgne, G. *et al*, *J. Organomet. Chem.*, 1977, **131**, 429 (*bibl*)
Seyferth, D. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 508 (*synth*)
Seyferth, D. *et al*, *Organometallics*, 1982, **1**, 125 (*synth*)
Matveev, V.V. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1987, 2616 (*mössbauer*)
Lagadec, A. *et al*, *J. Organomet. Chem.*, 1987, **326**, 381 (*synth*)
Darchen, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1988, 968 (*electrochem*)

$C_8H_6Fe_2O_6Se_2$ IC-005916

Hexacarbonylbis[μ-(methaneselenolato)]diiron, 9CI

[38497-97-1]



R = Me

M 467.7

syn-form

Air-stable ruby-red malodorous cryst. Mp 134-135° (84°).

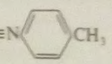
Rosenbuch, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1963 (*synth, pmr, ir*)
Seyferth, D. *et al*, *J. Organomet. Chem.*, 1981, **204**, 333 (*synth, pmr, ir*)
Seyferth, D. *et al*, *Organometallics*, 1986, **5**, 539 (*reaction*)

C_8H_7AgClN IC-005917

Chloro(1-isocyano-4-methylbenzene)silver

(*p-Tolylisocyanide*)*chlorosilver*

[41676-86-2]



M 260.4

Insol. common org. solvs. Mp 153-156° dec.

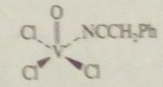
Minghetti, G. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 260 (*use*)
Minghetti, G. *et al*, *Inorg. Chem.*, 1975, **14**, 1974 (*synth*)

$C_8H_7Cl_3NOV$ IC-005918

(Benzeneacetonitrile)trichlorooxovanadium(*V*), 11CI

Trichlorooxo(phenylacetonitrile)vanadium(V). *Oxotrichloro(phenylacetonitrile)vanadium*(V). *Vanadium*(V) *oxychloride phenylacetonitrile*

[73165-10-3]



M 290.4

Square pyramidal. Synth. from $VOCl_3$ + $PhCH_2CN$.

Black solid. See also (Benzonitrile) trichlorooxovanadium(*V*), IC-005692.

Gourdon, A. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 304 (*synth, cryst struct*)

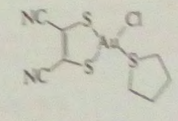
IC-005919

$C_8H_8AuClN_2S_3$

Chloro(maleonitriledithiolato)(tetrahydrothiophene) gold(*III*)

Chloro[2,3-dimercapto-2-butenedinitrilato(2−)-S,S′] (tetrahydrothiophene)gold, 11CI

[80316-71-8]



M 460.7
Green cryst. (CH_2Cl_2/Et_2O). Mp 181° dec.

Usón, R. *et al, Inorg. Chim. Acta*, 1981, **52**, 29 (*synth*)

IC-005920

C_8H_8AuNOS

Aurothioglycanide, INN
(2-Mercaptoanilidato-S)gold. Lauron. [[(*Phenylcarbamoyl*)*methyl*]*thio*]*gold*(I)
[16925-51-2]

$PhNHCOCH_2SAu$

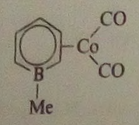
M 363.1
Antiarthritic agent. Greyish-yellow powder. Insol. most solvs. Mp 238-241°. Used as suspension in sesame oil.

U.S. Pat., 2 451 841, (1948); *CA*, 1913, **43** (*synth, pharmacol*)
Margolis, H.M. *et al, Am. J. Med. Sci.*, 1949, **218**, 121; *CA*, **44**, 3154 (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 5295.

IC-005921

$C_8H_8BCoO_2$

Dicarbonyl(1-methylborinato)cobalt
Dicarbonyl[*methyl*(η^5-*1,3-pentadien-1-yl-5-ylidene*)*borato*(1−)-B]*cobalt*, *11CI*. (η^6-*1-Methyl-1-boratabenzene*)*dicarbonylcobalt*
[95407-78-6]



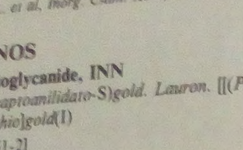
M 205.8
Sl. air-sensitive red-brown oil. Sol. Me_2CO. $Bp_{0.00001}$ 30°. ^{11}B nmr δ 23.2.

Herberich, G.E. *et al, J. Organomet. Chem.*, 1985, **280**, 147 (*synth, nmr, ms, ir*)
Böhm, M.C. *et al, J. Phys. Chem.*, 1985, **89**, 2129.

IC-005922

$C_8H_8Br_2CdN_4S_2$

Dibromobis[2(1*H*)-pyrimidinethione-N^3,S^2]cadmium, 10CI
Bis[*2*(*1H*)-*pyrimidinethione*]*cadmium dibromide*
[68193-91-9]



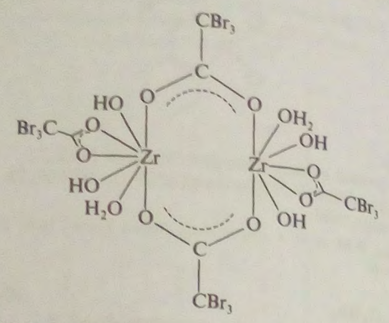
M 496.5
Pale yellow cryst. Sol. DMSO; insol. Et_2O, EtOH. Dichloro and diiodo analogues also prepared.
[88194-65-4]

Abbott, J. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 880 (*synth*)
Shunmugam, R. *et al, Indian J. Chem., Sect. A*, 1983, **22**, 784 (*pmr, cmr*)

IC-005923

$C_8H_8Br_{12}O_{14}Zr_2$

Diaquatetrahydroxybis[μ-(tribromoacetato-*O*,*O*′)]bis(tribromoacetato-*O*,*O*′)dizirconium(*IV*), 11CI
Aquadihydroxybis(*tribromoacetato*)*zirconium*(IV) *dimer*
[98776-59-1]



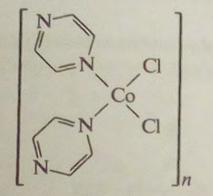
M 1469.4
Tentative struct. shown. Synth. by adding an aq. soln. of $ZrOCl_2.8H_2O$ to aq. tribromoacetic acid and heating. White solid. Insol. H_2O.

Patel, N. *et al, J. Less-Common Met.*, 1985, **109**, 361 (*synth, ir, thermal anal*)

IC-005924

$C_8H_8Cl_2CoN_4$

Dichlorobis(pyrazine)cobalt(*II*)



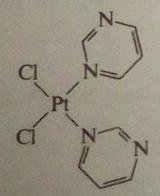
M 290.0
Octahedral polymeric struct. Many similar complexes also synth. Pink cryst. Sol. Me_2CO. Paramagnetic.

Lever, A.B.P. *et al, J. Chem. Soc.*, 1962, 1235 (*synth, uv, magnetism, ir*)

IC-005925

$C_8H_8Cl_2N_4Pt$

Dichlorobis(pyrimidine)platinum(*II*), 10CI



cis-form

M 426.1

cis-form [77309-61-6]
Early structural assignment was incorrect: pyrimidine acts as a monodentate ligand. Synth. from $PtCl_4^{2\ominus}$ and pyrimidine. Yellow solid. Sol. H_2O, polar solvs.

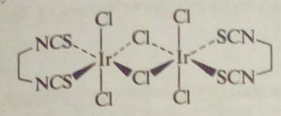
trans-form [77397-71-8]
Prepared from *cis*-form by crystallisation from DMF or DMSO. Yellow solid.

Kong, P.C. *et al, Can. J. Chem.*, 1979, **57**, 526 (*synth*)
Rochon, F.D. *et al, Can. J. Chem.*, 1981, **59**, 195 (*synth, cryst struct*)

IC-005926

$C_8H_8Cl_6Ir_2N_4S_4$

Di-μ-chlorotetrachlorobis(1,2-dithiocyanatoethane)diiridium(*III*)
Di-μ-chlorotetrachlorotetrakis(*thiocyanic acid*)*diiridium cyclic diethylene ester*, *8CI*



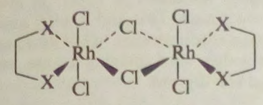
M 885.5
Bioctahedral, dimer cleaved by monodentate ligands. Pale yellow microcryst. Dec. at >250°.

Goodall, D.C., *J. Chem. Soc. A*, 1967, 203 (*synth, ir*)

IC-005927

$C_8H_8Cl_6N_4Rh_2S_4$

Di-μ-chlorotetrachlorobis(1,2-dithiocyanatoethane-*S*,*S*′)dirhodium(*III*)
Di-μ-chlorotetrachlorotetrakis(*thiocyanic acid*)*dirhodium*, *bis*(*cyclic ethylene*) *ester*, *8CI*
[15381-09-6]



X = NCS

M 706.9
Formed from $RhCl_3.3H_2O$ and 1,2-dithiocyanatoethane in 2-methoxyethanol. Light brown microcryst. Dec. >250°.

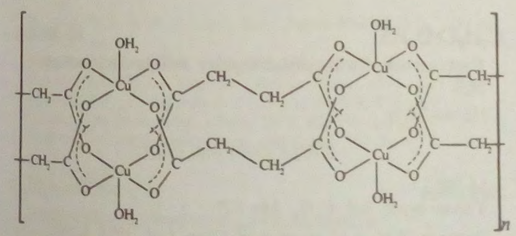
Monomer:
$C_4H_4Cl_3N_2RhS_2$ M 353.4

Goodall, D.C., *J. Chem. Soc. A*, 1967, 203 (*synth, ir*)

IC-005928

$C_8H_8Cu_2O_8$

Bis[μ-[butanedioato(2−)-*O*,*O*‴:*O*′,*O*″]]dicopper, 10CI
Copper(II) *succinate dimer*
[73613-63-5]



dihydrate

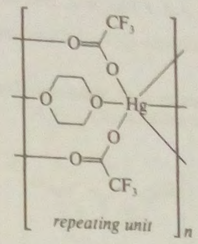
M 359.2
Light or dark blue solid. μ_{eff} = 1.39μ_B (r.t.).
Dihydrate: [55326-78-8]. *Diaquabis*[*μ*-[*butanedioato*(2−)-O,O‴:O′,O″]]*dicopper*
Blue cryst. Cu—Cu 257 pm.

Asai, O. *et al, J. Phys. Chem.*, 1959, **63**, 96 (*magnetism, hydrate*)
O'Conner, B.J. *et al, Acta Crystallogr.*, 1966, **20**, 824 (*hydrate, cryst struct, synth*)
Jasien, P.G. *et al, J. Inorg. Nucl. Chem.*, 1980, **42**, 924 (*synth, magnetism*)

IC-005929

$C_8H_8F_6HgO_6$

(Dioxane-O^1,O^4)bis(trifluoroacetato-*O*)mercury
(*Dioxane*)*mercury bis*(*trifluoroacetate*)
[84412-55-5]



M 514.7
Contains 6-coordinate Hg in the solid state. Cryst. (CH_2Cl_2 or Et_2O). Mp 139-140° dec.
[72622-21-0]

Boev, V.I., *J. Gen. Chem. USSR* (*Engl. Transl.*), 1979, **49**, 2505 (*synth*)
Small, R.W.H., *Acta Crystallogr., Sect. B*, 1982, **38**, 2886 (*synth, cryst struct*)

IC-005930

$C_8H_8HgO_2S$

(Acetato-*O*,*O*′)(benzenethiolato)mercury
[106371-06-6]

HgOAc(SPh)

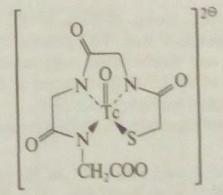
M 368.8
Infinite S—Hg—S chains are linked via acetate groups into sheets; Hg(1) 5 coord. (2S + 3O), Hg(2) 6 coord. (2S + 4O) in solid state. Synth. from $Hg(OAc)_2$ and $Hg(SPh)_2$ in MeCN soln. Cryst. (MeCN).

Stalhandska, C.I. *et al, Acta Crystallogr., Sect. C*, 1986, **42**, 1731 (*synth, cryst struct*)

IC-005931

$C_8H_8N_3O_6STc^{2\ominus}$

[*N*-[*N*-[*N*-(Mercaptoacetyl)glycyl]glycyl]glycinato(5−)-*N*,*N*′,*N*″,*S*]oxotechnetate(2−), 12CI
Mercaptoacetyltriglycine-Tc. *MAG*$_3$*-Tc*. *Tc-MAG*$_3$. *Tc-mertiatide*
[104318-29-8]



M 373.1 (ion)
This N_3S ligand gives a Tc complex analogous to the diaminodithiolato (N_2S_2) series, but without the latter's stereochemical complications. Several other mercaptotripeptide ligand-Tc complexes have been prepared, but none are yet of any importance. Synth. from $TcO_4^{\ominus}$ plus preformed ligand with dithionite reduction, or by ligand exchange from Tc gluconate complex. Renal imaging agent; no clear advantage over widely used Tc-DTPA; clinical preparations have limited shelf-life.

[104348-91-6, 104758-54-5]

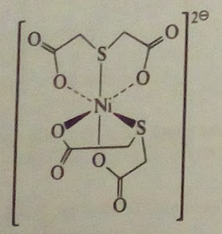
Fritzberg, A.R. *et al*, *J. Nucl. Med.*, 1986, **27**, 111 (*synth*)
Taylor, A. *et al*, *Radiology*, 1987, **162**, 365 (*pharmacokinetics*)
Taylor, A. *et al*, *J. Nucl. Med.*, 1988, **29**, 616 (*synth, biodistribn*)
Brandau, W. *et al*, *Nuklearmedizin, Suppl. (Stuttgart)*, 1988, **24**, 748 (*synth, biodistribn*)
Bannister, K.M. *et al*, *J. Nucl. Med.*, 1990, **31**, 1568 (*synth, biodistribn*)

$C_8H_8NiO_8S_2^{2\ominus}$ IC-005932

Bis[thiobis(acetato)-*O,O',S*]nickelate(*II*)(2−), 9CI

Bis(thiodiacetato)nickelate(II)(2−), *8CI*

[31340-57-5]



M 354.9 (ion)
Octahedral. Dec. in H_2O.

fac,cis-form

Na salt, octahydrate: [31117-86-9].
$C_8H_{24}Na_2NiO_{16}S_2$ M 545.0
Blue solid.

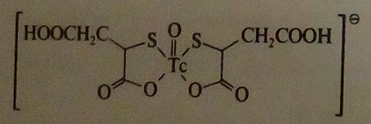
K salt, trihydrate: [60497-55-4].
$C_8H_{14}K_2NiO_{11}S_2$ M 487.2
Blue prisms.

Podlahova, J., *Inorg. Chim. Acta*, 1970, **4**, 549 (*synth, ir, uv, dta*)
Delaunay, J. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 2341 (*synth, cryst struct*)

$C_8H_8O_9S_2Tc^{\ominus}$ IC-005933

Bis[2-mercaptobutanedioato(2−)-*O,S*]oxotechnetate(*V*) (1−)

Bis(thiomalato)oxotechnetate(V)



M 411.1 (ion)
Speculative struct. shown; ill-characterised complex, though preparation from $TcO(gluconate)_2$ suggests oxdn. state and stoichiometry assumed here. Synth. e.g. by reaction of $TcO_4^{\ominus}$ with an excess of thiomalate. Also synth. by ligand exchange with bis-gluconatooxotechnetate(*V*). Promising imaging agent for the liver.

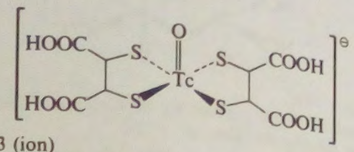
Hagan, P.L. *et al*, *J. Nucl. Med.*, 1975, **16**, 531 (*synth*)
Ikeda, I. *et al*, *Int. J. Appl. Radiat. Isot.*, 1977, **28**, 387 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, *Suppl. Vol.* 2, 1983, 235 (*bibl*)

$C_8H_8O_9S_4Tc^{\ominus}$ IC-005934

Bis[2,3-dimercapto-1,4-butanedioato(2−)-*S,S'*]oxotechnetate(1−)

Bis[2,3-dimercaptobutanedioato(4−)-S,S']oxotechnetate(5−), tetrahydrogen, 12CI.
Bis(dimercaptosuccinato)oxotechnetate(V). *Succimer-Tc*

[82711-85-1]



M 475.3 (ion)
Square-pyramidal anion; ligand in *meso-* or *rac*-form (or as dimethyl ester). There have been suggestions of *O,O' vice S,S'* coordination. It is often unclear whether Tc(*III*) (Tris[2,3-dimercaptobutanedioato(2−)-*O,O'*]technetate(3−), IC-007607) or Tc(*V*) complex is involved in pharmacol. applications, but this oxotechnate(*V*) form has recently been fully characterised. Synth. from $TcO(gluconate)_2$, or by Sn(*II*) or electrochem. reduction of $TcO_4^{\ominus}$ in presence of 2,3-dimercaptosuccinate. This and Tc(*III*) analogue Tris[2,3-dimercaptobutanedioato(2−)-*O,O'*]technetate(3−), IC-007607 are widely used imaging agents, especially for kidneys and for thyroid.

(±,±)-form
rac-*form*

Et_4N salt: Red solid ($MeNO_2$). Mp 200-204°.
Tetrabutylammonium salt: Orange-red needles. Spar. sol. H_2O.

[65438-08-6, 125295-31-0]

Lin, T.H. *et al*, *J. Nucl. Med.*, 1974, **15**, 34.
Spies, H. *et al*, *Inorg. Chim. Acta*, 1981, **48**, 255 (*synth, uv, ir, pmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, *Suppl. Vol.*, 1983, **2**, 234 (*rev, bibl*)
Chatterton, B.E. *et al*, *Aust. N.Z. J. Med.*, 1987, **17**, 480 (*biodistribn*)
Clarke, S.E.M. *et al*, *J. Nucl. Med.*, 1988, **29**, 33 (*pharmacol*)
DeGregori, I. *et al*, *Appl. Radiat. Isot.*, 1989, **40**, 385 (*synth, uv, ir, electrochem*)

$C_8H_9CrO_5PS$ IC-005935

Pentacarbonyl(trimethylphosphine sulfide-*S*)chromium, 9CI

[35244-74-7]

$(OC)_5CrS{=}PMe_3$ (C_{4v})

M 300.1
Yellow cryst. Sol. C_6H_6. Mp 87°.

Doorman, B.M. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 941.
Baker, E.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2205 (*cryst struct*)
Ainscough, E.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2360 (*synth, props*)
Raubenheimer, H.G. *et al*, *J. Organomet. Chem.*, 1976, **112**, 145 (*ir*)

$C_8H_9GeMnO_5$ IC-005936

Pentacarbonyl(trimethylgermyl)manganese, 9CI

[37843-69-9]

$Me_3GeMn(CO)_5$

M 312.7

Synth. from Me_3GeBr and $Na[Mn(CO)_5]$ in THF. Colourless cryst. Mp 33.5-34.5°. Subl.$_{0.001}$ 25°. Ir ν_{CO} 2117m, 2030vs, 2000s cm^{-1} (nujol).

Clark, H.C. *et al*, *Inorg. Chem.*, 1966, **5**, 1582 (*synth, pmr, ir*)
Burnham, R.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1269 (*ir, ms, raman*)
McLean, R.A.N., *J. Chem. Soc., Dalton Trans.*, 1974, 1568 (*uv*)

$C_8H_9MnO_5Pb$ IC-005937

Pentacarbonyl(trimethylplumbyl)manganese, 9CI

(Trimethylplumbyl)pentacarbonylmanganese

[36527-71-6]

$Me_3PbMn(CO)_5$

M 447.2
Synth. from Me_3PbCl and $Na[Mn(CO)_5]$ in THF. Fairly air-stable yellow cryst. (pet. ether), slowly dec. in org. solvs. Readily sol. polar solvs., mod. sol. EtOH, C_6H_6. Mp 30-31°. Bp 60-62°. Disproportionates in THF soln. to Me_4Pb and Bis(pentacarbonylmanganese) dimethyllead, IC-007424.

[25880-34-6]

Gorsich, R.D., *J. Am. Chem. Soc.*, 1962, **84**, 2486 (*synth, props*)
Jetz, W. *et al*, *Inorg. Chem.*, 1966, **5**, 2217 (*pmr*)
Kahn, O. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, **266**, 792 (*ir*)
Haupt, H.J. *et al*, *J. Organomet. Chem.*, 1973, **54**, 231 (*synth*)
Kodel, W. *et al*, *Inorg. Chim. Acta*, 1981, **49**, 209.

$C_8H_9MnO_5Si$ IC-005938

Pentacarbonyl(trimethylsilyl)manganese, 9CI, 8CI

Trimethylsilylmanganese pentacarbonyl

[26500-16-3]

$Me_3SiMn(CO)_5$

M 268.1
Synth. from Me_3SiCl and $Na[Mn(CO)_5]$ in THF. Air-sensitive, volatile, thermally-stable white cryst. Mp 25.6-26.2°. Ir ν_{CO} 2094w, 2000s, 1993vs cm^{-1} (cyclohexane).

Hamilton, R.S. *et al*, *Diss. Abstr. B*, 1968, **29**, 1595 (*struct*)
Berry, A.D. *et al*, *Inorg. Nucl. Chem. Lett.*, 1969, **5**, 601 (*synth, ir, pmr*)
Burnham, R.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1269 (*ir, raman, ms*)
Malisch, W. *et al*, *Chem. Ber.*, 1974, **107**, 979 (*synth, ir*)
McLean, R.A.N., *J. Chem. Soc., Dalton Trans.*, 1974, 1568 (*uv*)
Spalding, T.R., *J. Organomet. Chem.*, 1978, **149**, 371 (*ms*)
Gladysz, J.A. *et al*, *Inorg. Chem.*, 1979, **18**, 553 (*synth*)
Li, S. *et al*, *J. Organomet. Chem.*, 1979, **166**, 317 (*nmr*)

$C_8H_9MnO_5Sn$ IC-005939

Pentacarbonyl(trimethylstannyl)manganese

[14126-94-4]

$Me_3SnMn(CO)_5$

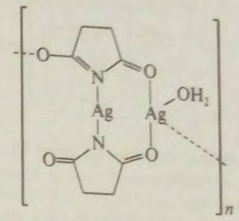
M 358.8
Synth. from Me_3SnCl and $Na[Mn(CO)_5]$ in THF. White cryst. (pentane). Mp 26-27°. Subl. 0° *in vacuo*. Ir ν_{CO} 2089, 1998, 1991 cm^{-1} (cyclohexane).

Jetz, W. *et al*, *Inorg. Chem.*, 1966, **5**, 2217 (*synth, ir, pmr*)
Bryan, R.F., *J. Chem. Soc. A*, 1968, 696 (*struct*)
Onaka, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 726 (*mössbauer, Mn-55 nmr*)
Burnham, R.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1269 (*ir, raman, ms*)
Roberts, R.M.G., *J. Organomet. Chem.*, 1973, **47**, 359 (*synth*)
McLean, R.A.N., *J. Chem. Soc., Dalton Trans.*, 1974, 1568 (*uv*)
Harris, D.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 311 (*Sn-119 nmr*)
Avazino, S.C. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1976, **8**, 15 (*pe*)

$C_8H_{10}Ag_2N_2O_5$ IC-005940

Aqua(μ$_3$-succinimidato-*N:O:O'*)(μ-succinimidato-*N:O*)disilver(*I*)

[91191-42-3]



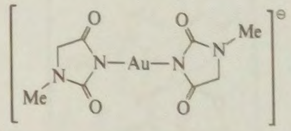
M 429.9
Polymeric struct. Greyish solid. Mp 250° dec. Ir ν_{OH_2} 3640, 3540; ν_{CO} 1650 cm^{-1} (MeCN).

Ley, H. *et al*, *Ber. Dtsch. Chem. Ges.*, 1906, **39**, 1259 (*synth*)
Huot, J.Y. *et al*, *Can. J. Chem.*, 1983, **61**, 1890 (*synth, electrochem, uv, ir, pmr*)
Perron, J. *et al*, *Inorg. Chem.*, 1984, **23**, 2853 (*electrochem, cryst struct, ir, pmr, cmr*)

$C_8H_{10}AuN_4O_4^{\ominus}$ IC-005941

Bis(*N*^{3}-methylimidazolidinedionato-*N*^{1})aurate(1−)

Bis(N-*methylhydantoinato*)*gold*(1)



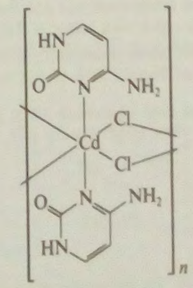
M 423.1 (ion)
Na salt, tetrahydrate: Colourless cryst. (H_2O). Mp 216-218°.

Malik, N.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1978, 711 (*synth, cryst struct, pmr, ir, mössbauer*)

$C_8H_{10}CdCl_2N_6O_2$ IC-005942

Dichlorobis(cytosine)cadmium

Bis[4-*amino*-2(1*H*)-*pyrimidinone*-N^3]*dichlorocadmium, 12CI*



M 405.5
Presumed octahedral polymeric struct. shown. White solid (H_2O); completely dissoc. in H_2O. Sol. DMSO. Forms several hydrates.

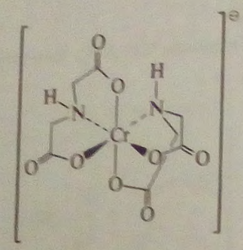
Pizzino, T. *et al*, *Monatsh. Chem.*, 1990, **121**, 3 (*synth, ir, thermal anal, pmr, cmr, uv-vis, props*)

IC-005943

$C_8H_{10}CrN_2O_8^{\ominus}$

Bis(iminodiacetato)chromate(*III*)(1−)

Bis[N-(*carboxymethyl*)*glycinato*(2−)-N,O,O^{x}]*chromate*(III) (*1−*), *10CI*



M 314.1 (ion)

Distorted octahedral coordination about Cr, with the N atoms in a *cis* config.

K salt: [73190-73-5].

Deep red prisms + $3H_2O$ (H_2O).

[21417-70-9, 25862-75-3]

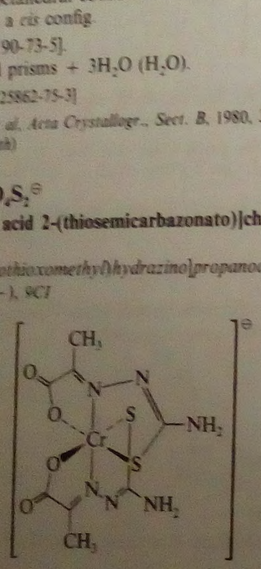
Mootz, D. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 445 (*cryst struct, synth*)

IC-005944

$C_8H_{10}CrN_4O_4S_2^{\ominus}$

Bis[pyruvic acid 2-(thiosemicarbazonato)]chromate(*III*) (1−), 8CI

Bis[2-[(*aminothioxomethyl*)*hydrazino*]*propanoato*(2−)] *chromate*(*1−*), *9CI*



M 370.3 (ion)

mer-Octahedral.

NH_4 salt: [31006-59-4].

Synth. from Cr(*III*) salt, conc. NH_3 and pyruvic acid thiosemicarbazone. Brown plates. Sol. H_2O; less sol. MeOH, EtOH; insol. Et_2O, Me_2CO. μ_{eff} = 3.76μ_B.

Ba salt (2:1): [35861-16-6].

Synth. from the ammonium salt and $BaCl_2.2H_2O$. Elongated dark red-brown plates + $5H_2O$.

Ablov, A.V. *et al*, *Zh. Neorg. Khim.*, 1970, **15**, 1854; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1970, **15**, 952 (*synth, magnetism, struct*)

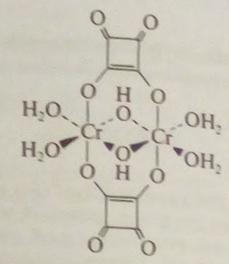
Volodina, G.F. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1971, **200**, 1349; *Dokl. Chem.* (*Engl. Transl.*), 1971, **200**, 853 (*cryst struct*)

$C_8H_{10}Cr_2O_{14}$ IC-005945

Tetraaquabis[μ-[3,4-dihydroxy-3-cyclobutene-1,2-dionato(2−)-O^3:O^4]]di-μ-hydroxydichromium(*III*), 10CI

Tetraaquadi-μ-hydroxobis(*μ-cyclobut-3-ene-1,2-dione-3,4-diolato*-O,O′)*dichromium. Tetraaquadi-μ-hydroxobis*(*μ-squarato*-O,O′)*dichromium*(III)

[77974-14-2]



M 434.1

Cryst. + $2H_2O$.

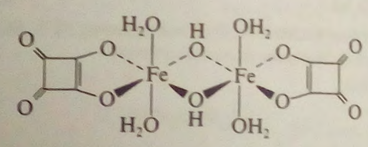
Chesick, J.P. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 1076 (*cryst struct, synth*)

$C_8H_{10}Fe_2O_{14}$ IC-005946

Tetraaquabis[3,4-dihydroxy-3-cyclobutene-1,2-dionato(2−)-O^3,O^4]di-μ-hydroxydiiron, 9CI

Tetraaquadi-μ-hydroxybis(*squarato*)*diiron*(III)

[67424-50-4]



M 441.8

Synth. from $Fe(NO_3)_3$ (hydrated) + $C_4O_4H_2$ in H_2O. Stable, black-violet cryst; also reported as dark brown powder. Forms a dihydrate. Shows antiferromagnetic exchange coupling.

[66540-74-7]

West, R. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 2589 (*synth, magnetism*)

Condren, S.M. *et al*, *Inorg. Chem.*, 1973, **12**, 57 (*related system*)

Long, G., *Inorg. Chem.*, 1978, **17**, 2702 (*mössbauer, ir, uv-vis, magnetism, struct*)

Wrobleski, J.T. *et al*, *Inorg. Chem.*, 1978, **17**, 2959 (*synth, magnetism, mössbauer, ir*)

Wrobleski, J.T. *et al*, *Inorg. Chim. Acta*, 1979, **35**, 109 (*reactivity*)

Long, G.J. *et al*, *Inorg. Chim. Acta*, 1981, **54**, L117 (*mössbauer*)

$C_8H_{10}NS_7Zn^{\ominus}$ IC-005947

(*N,N*-Diethyldithiocarbamato-*S,S′*)[4,5-dimercapto-1,3-dithiole-2-thionato(2−)-S^4,S^5]zincate(1−)

(*Diethylcarbamodithioato*-S,S′)[*4,5-dimercapto-1,3-dithiole-2-thionato*(2−)-S^4,S^5]*zincate*(*1−*)

M 410.0 (ion)

Approx. tetrahedral at Zn.

Tetrabutylammonium salt: [128494-27-9].

Orange cryst. (heptane/2-propanol or EtOH/Me_2CO). Sol. DMSO. Mp 89-91°.

Dietzsch, W. *et al*, *Inorg. Chim. Acta*, 1990, **169**, 55 (*synth, cmr, pmr, cryst struct*)

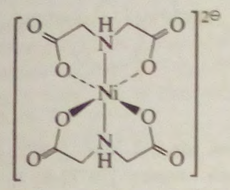
IC-005948

$C_8H_{10}N_2NiO_8^{2\ominus}$

Bis(iminodiacetato)nickelate(*II*)(2−), 8CI

Bis[N-(*carboxymethyl*)*glycinato*-N,O,O′]*nickelate*(II)(*2−*), *9CI*

[23314-44-5]



M 320.8 (ion)

Octahedral.

trans-form

Di-Li salt, tetrahydrate: [52646-82-9].

Blue needles. Ir ν_{NH} 3235-3280; ν_{COO} 1415 cm^{-1}.

Di-Na salt, heptahydrate: [26009-89-2].

Light purple cryst. Ir ν_{NH} 3300s; ν_{COO} 1400vs; ν_{CN} 1110m, 1080m cm^{-1} (KBr). Dehydrated >98°; μ_{eff} = 3.15 μ_B.

Di-Cs salt, tetrahydrate: [62661-01-2].

Blue prisms.

Laitinen, S. *et al*, *Suom. Kem. B*, 1970, **43**, 61; *CA*, **72**, 96164s (*synth, ir, uv*)

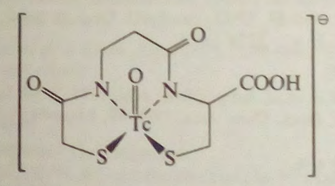
Mammano, N.J. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 1251 (*synth, cryst struct*)

Lukes, I. *et al*, *Inorg. Chim. Acta*, 1983, **76**, L99 (*synth, ir, uv*)

$C_8H_{10}N_2O_5S_2Tc^{\ominus}$ IC-005949

[8-Carboxylato-1,9-dimercapto-2,6-dioxo-3,7-diazanonanato]oxotechnetate(*V*)(1−)

Tc—CAP—DADS. CAP—DADS—Tc



M 377.2 (ion)

Synth. from $TcO_4^{\ominus}$ + preformed ligand, with $SnCl_2$ reduction. Promising agent for renal imaging; carboxylato-substits. seem to confer favourable props.

Schneider, R.F. *et al*, *J. Nucl. Med.*, 1984, **25**, 223 (*ligand synth*)

McAfee, J.G. *et al*, *J. Nucl. Med.*, 1985, **26**, 375 (*synth, biodistrib*)

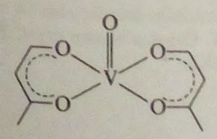
$C_8H_{10}O_5V$ IC-005950

Oxobis(3-oxobutanalato-*O,O′*)vanadium(*IV*), 11CI

Bis(*acetoacetaldehydato*)*oxovanadium*(IV).

Bis(*formylacetonato*)*oxovanadium*(IV)

[99351-16-3]



M 237.1

Synth. from $VOSO_4$ and ligand. May be used as catalyst for ethylene/propylene copolym.

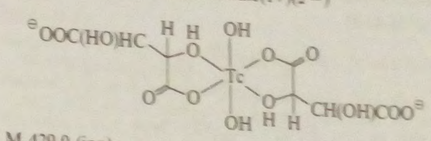
Mehrotra, R.C. *et al*, *Metal Complexes and Allied Derivatives*, Academic Press, London, 1978 (*synth*)

Milani, F. *et al*, *Inorg. Chim. Acta*, 1985, **103**, 15 (*use*)

$C_8H_{10}O_{14}Tc^{2\ominus}$ IC-005951

Dihydroxybis(tartrato)technetate(*IV*)(2−)

Bis-tartrato-bis-hydroxotechnetate(IV)(*2−*)



M 429.0 (ion)

Suggested struct. shown. Several other Tc(*IV*) tartrate species, and one Tc(*V*) tartrate, have been proposed. Synth. from $TcBr_6^{2\ominus}$ and tartrate. Examined as bone imaging agent.

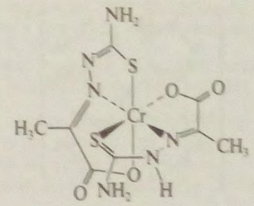
Technetium in Chemistry and Nuclear Medicine, (Ed. Deutsch, E., *et al*), Cortina International, Verona, 1983, 39, 51.

$C_8H_{11}CrN_5O_4S_2$ IC-005952

Bis(pyruvic acid thiosemicarbazonato-*N,O,S*) chromium(*III*)

[2-[(*Aminothioxomethyl*)*hydrazono*]*propanoato*][2-[(*aminothioxomethyl*)*hydrazono*]*propanoato*(2−)] *chromium*(III), *11CI*

[97995-60-3]



M 371.3

Cr is coordinated by two deprotonated forms of pyruvic acid thiosemicarbazone, appreciably distorted from ideal octahedral geometry. Dark purple cryst. + $1H_2O$.

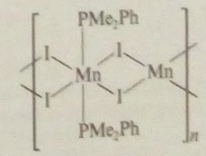
Timken, M.D. *et al*, *Inorg. Chem.*, 1985, **24**, 3450 (*cryst struct, synth, ir*)

IC-005953

$C_8H_{11}I_2MnP$

(Dimethylphenylphosphine)diiodomanganese(*II*), 11CI

[71957-11-4]



M 446.8

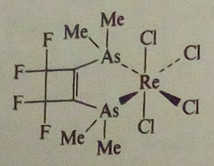
Contains alternating octahedral and tetrahedral Mn in a polymeric chain struct. Synth. from MnI_2 and PMe_2Ph in dry, oxygen free solvs. Pale orange cryst. Reversibly binds dioxygen to give green $MnI_2(PMe_2Ph)O_2$.

Brown, R.M. *et al*, *J. Organomet. Chem.*, 1980, **201**, 437.

McAuliffe, C.A., *J. Organomet. Chem.*, 1982, **228**, 255 (*synth, reaction*)
Beagley, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1984, 305 (*cryst struct*)

$C_8H_{12}As_2Cl_4F_4Re$ IC-005954

[1,2-Bis(dimethylarsino)-3,3,4,4-tetrafluoro-1-cyclobutene]tetrachlororhenium(*IV*)
Tetrachloro[(3,3,4,4-tetrafluoro-1-cyclobutene-1,2-diyl)bis(dimethylarsine)-As,As′]rhenium(IV), *9CI*
[54736-41-3]

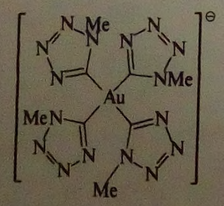


M 662.0
Synth. from $ReCl_5$ and ligand in CCl_4 or from $KReO_4$, HCl aq., H_3PO_2 aq. and ligand. Light green gelatinous solid or green cryst.

Maslen, E.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2128 (*synth, cryst struct*)
Kepert, D.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1903 (*synth, ir, w, props*)

$C_8H_{12}AuN_{16}^{\ominus}$ IC-005955

Tetrakis(1-methyl-1*H*-tetrazol-5-yl)aurate(1−), 8CI
Tetrakis(1-methyl-5-tetrazolato)aurate(1−)
[33461-24-4]



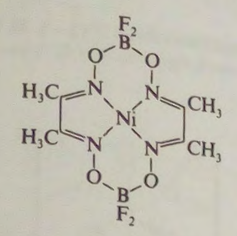
M 529.2 (ion)
Au(III) complex with four carbeniate ligands. Cryst. struct determination is on closely related isopropyl compd.
Tetraphenylarsonium salt:
$C_{32}H_{32}AsAuN_{16}$ M 912.6
Air-stable cryst. (CH_2Cl_2/Et_2O). Sol. CH_2Cl_2, $CHCl_3$, Me_2CO, spar. sol. THF, insol. Et_2O.

Beck, W. *et al*, *Chem. Ber.*, 1972, **104**, 1816 (*synth*)
Fehlhammer, W.P. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 3370 (*cryst struct*)

$C_8H_{12}B_2F_4N_4NiO_4$

Bis(difluoroborodimethylglyoxime)nickel(*II*) IC-005956

[*Bis*[*μ*-(2,3-butanedione dioximato)(2−)-O:O′]tetrafluorodiborato-N,N′:N″,N‴]*nickel*, *9CI*
[35200-43-2]



M 384.5
Yellow solid. Sol. Me_2CO. Subl. >300°. Dec. at 350°.
1H-Benzimidazole complex: [76772-41-3].
$C_{15}H_{18}B_2F_4N_6NiO_4$ M 502.6
Dark-amber diamond-shaped plates.
PPh_3 complex:
$C_{26}H_{27}B_2F_4N_4NiO_4P$ M 646.8
Brown cryst. (pet. ether). Mp 95°.

Schrauzer, G.N., *Chem. Ber.*, 1962, **95**, 1438 (*synth, uv, ir, deriv*)
Stephens, F.S. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 3159 (*cryst. struct*)
Stephens, F.S. *et al*, *Inorg. Chim. Acta*, 1980, **43**, 77 (*cryst struct, deriv*)
Beaumont, P.L. *et al*, *Inorg. Chim. Acta*, 1980, **45**, 99 (*ms*)
Gagné, R.R. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 1444.
Gagné, R.R. *et al*, *Inorg. Chem.*, 1981, **20**, 1991 (*ir*)

$C_8H_{12}Br_2N_4Ru$ IC-005957

Tetrakis(acetonitrile)dibromoruthenium(*II*), 9CI
Dibromotetrakis(ethanenitrile)ruthenium(II)
[50723-44-9]

$$Ru(N{\equiv}CCH_3)_4Br_2$$

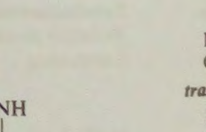
M 425.0
trans-Octahedral. Prepd. by reducing '$RuBr_3.xH_2O$' in MeCN with H_2 (PtO_2 catalyst). Orange solid. Sol. MeCN. Ir ν_{CN} 2278 cm^{-1}.

[96613-17-1]

Newton, W.E. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 349 (*synth, ir*)
Riley, D.P., *Inorg. Chim. Acta*, 1985, **99**, 5 (*synth*)

$C_8H_{12}Br_2N_4V^{\oplus}$ IC-005958

Tetrakis(acetonitrile)dibromovanadium(*III*)(1+), 11CI
Dibromotetrakis(methyl cyanide)vanadium(III)(*1+*)



M 374.9 (ion)
Octahedral.

trans-form

Tribromide: [103664-47-7].
Synth. by electrolysis of a MeCN soln. of Bu_4NBr and Br_2 using a vanadium anode; also by direct bromination of V in MeCN. Orange-brown cryst. Paramagnetic; μ_{eff} = 2.65μ_B (298K).

Hathaway, B.J. *et al*, *J. Chem. Soc.*, 1965, 537 (*synth, uv-vis, ir, magnetism*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1986, **25**, 3528 (*synth, cryst struct*)

$C_8H_{12}Br_4N_4U$ IC-005959

Tetrakis(acetonitrile)tetrabromouranium(*IV*)
[17499-65-9]

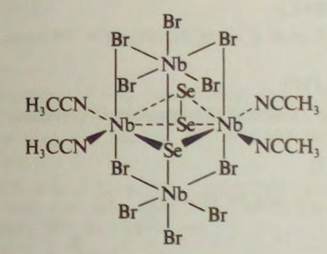
$$(MeCN)_4UBr_4$$

M 721.8
Useful starting material for synth. of UBr_4 compds. Deliquescent blue-grey cryst. Loses MeCN *in vacuo* >40°. Paramagnetic, μ_{eff} = 2.78 μ_B (298K), θ −148°.

Bagnall, K.W. *et al*, *J. Chem. Soc. A*, 1966, 1763 (*synth, ir*)
Inorg. Synth., 1970, **12**, 227 (*synth*)
du Preez, J.G.H. *et al*, *J. S. Afr. Chem. Inst.*, 1971, **24**, 135 (*synth*)
Gans, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 47 (*synth, uv, magnetism*)

$C_8H_{12}Br_{10}N_4Nb_4Se_3$ IC-005960

Tetrakis(acetonitrile)tetra-μ-bromohexabromo[μ-(diselenium-*Se,Se′:Se,Se′*)]-μ_4-selenoxotetraniobium(*III,IV*), 11CI
Tetra-μ-bromo(μ-diselenido)(μ_4-selenido)hexabromotetrakis(methyl cyanide)tetraniobium(III,IV)
[81984-99-8]

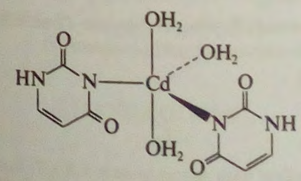


M 1571.7
Synth. from $NbBr_4.2MeCN$ and Sb_2Se_3 in MeCN. Cryst. Diamagnetic.

Benton, J.A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1981, 1241 (*synth, cryst struct*)

$C_8H_{12}CdN_4O_7$ IC-005961

Triaquabis(uracilato)cadmium
Triaquabis(2,4(1H,3H)-pyrimidinedionato-N^3)cadmium, *10CI*
[75575-81-4]



M 388.6
Trigonal bipyramidal with equatorial N-ligands. Cryst. (conc. aq. NH_3).

Mutikainen, I. *et al*, *Acta Crystallogr., Sect. B*, 1980, **36**, 2237 (*synth, cryst struct*)

$C_8H_{12}CdO_8^{2\ominus}$ IC-005962

Tetrakis(acetato-*O*)cadmate(2−)
[18747-51-8]

$$[Cd(OAc)_4]^{2\ominus}$$

M 348.5 (ion)
Di-Rb salt: [57128-10-6].
Cryst. Mp 206°.
Ca salt: [28849-56-1].
Cryst. + H_2O.

[32146-38-6]

Nazarovo, L.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1971, **16**, 1704 (*stability const*)
Nadirov, E.G. *et al*, *Tr. Khim.-Metall. Inst., Akad. Nauk Kaz. SSR*, 1974, **25**, 129 (*thermal anal, powder struct, synth, Rb salt*)
Kowalski, J. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1978, **52**, 2297 (*synth*)

$C_8H_{12}CeO_8$ IC-005963

Cerium(*IV*) acetate
Ceric acetate. Cerium tetraacetate
[19475-87-7]

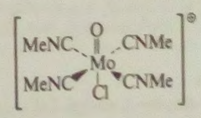
$$Ce(OAc)_4$$

M 376.2
Synth. by ozonolysis of Ce(*III*) acetate in presence of $NO_3^{\ominus}$. Useful org. reactant. Oxidises aldehydes and ketones at α-carbon. Used in synth. of arylacetic acids and lactones. Air and light sensitive hygroscopic bright yellow solid. Sl. sol. HOAc, C_6H_6; Sol. H_2O. Diamagnetic.

Patnaik, D. *et al*, *Curr. Sci.*, 1957, **26**, 355 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1062; 1974, **4**, 71 (*use*)
Hay, N.E. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 884 (*synth, uv-vis*)
Trahanovsky, W.S. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 5060, 5068 (*use*)
Heiba, E.I. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 995 (*use*)
U.S. Pat., 4 175 089, (1979); *CA*, **93**, 7666 (*use*)
U.S. Pat., 4 285 868, (1981); *CA*, **96**, 6196 (*use*)
Baciocchi, F. *et al*, *J. Chem. Res.* (*S*), 1983, 232 (*use*)

$C_8H_{12}ClMoN_4O^{\oplus}$ IC-005964

Chlorotetrakis(isocyanomethane)oxomolybdenum(*IV*) (1+), 9CI
Oxochlorotetrakis(methyl isocyanide)molybdenum(IV)(*1+*)



M 311.6 (ion)
Octahedral cation.

trans-form

Triiodide: [50432-36-5].
V. reactive towards amines + thiols. Fairly air-stable maroon red needles. Sol. $MeNO_2$; part. sol. MeCN. Dec. in Me_2CO or MeOH soln.
Hexafluorophosphate: [50432-35-4].
V. reactive towards amines and thiols. Fairly air-stable purple microcryst. Sol. $MeNO_2$; part. sol. MeCN; dec. in MeOH or Me_2CO soln. Diamagnetic.

Novotny, M. *et al*, *Inorg. Chem.*, 1974, **13**, 828 (*synth, props, ir*)
Lam, C.T. *et al*, *Inorg. Chem.*, 1976, **15**, 989 (*cryst struct*)

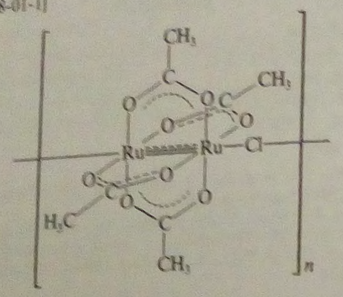
IC-005965

$C_8H_{12}ClO_8Ru_2$

Tetrakis[μ-(acetato-*O*:*O*′)]-μ-chlorodiruthenium, 9CI

catena-μ-Chlorotetra-μ-ethanoato-(O,O′)-diruthenium(III,II)

[55598-01-1]



M 473.7

An important structural type for a mixed-valence complex. Containing an infinite polymeric chain of dinuclear units Ru—Ru 228.7; Ru—Cl 257.7 pm. Prepd. by treating $RuCl_3.xH_2O$ with AcOH. An important reagent and catalyst. Brown solid. Insol. most common solvs., but sol. hot MeOH. μ_{eff} = 4.07μ_B (298K); 3.82μ_B (106K) (per dimeric unit).

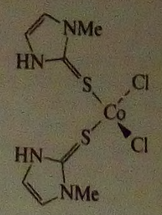
[38833-34-0]

Stephenson, T.A. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 2285 (*synth, magnetism*)
Bennett, M.J. *et al*, *Inorg. Chem.*, 1969, **8**, 1 (*ir*)
Clark, R.J.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1825 (*ir, raman*)
Bino, A. *et al*, *Inorg. Chem.*, 1979, **18**, 2599 (*cryst struct, related complexes*)
Norman, J.G. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 5256 (*theory*)
Togano, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 2085 (*cryst struct*)
Martin, D.S. *et al*, *Inorg. Chem.*, 1980, **19**, 3404 (*cryst struct, uv*)
Clark, R.J.H. *et al*, *Inorg. Chem.*, 1981, **20**, 2759 (*raman, uv*)
Seddon, E.A. *et al*, *The Chemistry of Ruthenium*, Elsevier, Amsterdam, 1984, 175 (*rev*)
Itagaki, H. *et al*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 2291 (*catalysis*)
Urbanos, F.A. *et al*, *Polyhedron*, 1988, **7**, 2597 (*synth*)
Cotton, F.A. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 6177 (*struct, bonding, reaction*)
Carvill, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1989, 2435 (*reaction*)
Keppler, B.K. *et al*, *Prog. Clin. Biochem. Med.*, 1989, **10**, 41 (*pharmacol*)
Collin, J.P. *et al*, *Inorg. Chem.*, 1990, **29**, 2238 (*reaction*)
Binamira-Soriaga, E. *et al*, *Inorg. Chem.*, 1990, **29**, 3167 (*reaction*)
Shin, K.S.K. *et al*, *J. Am. Chem. Soc.*, 1990, **112**, 7148 (*raman*)

$C_8H_{12}Cl_2CoN_4S_2$ IC-005966

Dichlorobis(1,3-dihydro-1-methyl-2*H*-imidazole-2-thione-*S*)cobalt(*II*), 10CI

[67168-26-7]



M 358.1

Prob. tetrahedral. Blue solid. Sol. $MeNO_2$, common org. solvs. Mp 180°. Paramagnetic.

Raper, E.S. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 2163 (*synth, ir, uv, magnetism*)

$C_8H_{12}Cl_2CrN_4$ IC-005967

Dichlorobis(1-methyl-1*H*-imidazole-N^3)chromium(*II*), 9CI

[58467-11-1]

$CrCl_2(C_4H_6N_2)_2$

M 287.1

Chloride-bridged polymer with distorted octahedral struct. Synth. from excess $CrCl_2$ + ligand in EtOH. Air-sensitive solid. Sol. DMF; insol. other common org. solvs. μ_{eff} = 4.69 (298K); 4.30μ_B (84K).

Mani, F. *et al*, *Inorg. Chim. Acta*, 1976, **16**, 163 (*synth, props*)

$C_8H_{12}Cl_2CrN_4$ IC-005968

Dichlorobis(1-methyl-1*H*-pyrazole-N^2)chromium(*II*), 10CI

[72950-80-2]

$CrCl_2(C_4H_6N_2)_2$

M 287.1

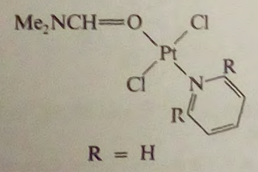
Halide-bridged polymer, config. not reported but prob. 6-coordinate by analogy with related compds. Synth. from $CrCl_2.4H_2O$ + ligand. Air-sensitive. μ_{eff} = 4.74 (295K), 4.46μ_B (84K).

Dapporto, P. *et al*, *J. Chem. Res. (S)*, 1979, 374 (*synth, props*)

$C_8H_{12}Cl_2N_2OPt$ IC-005969

Dichloro(*N*,*N*-dimethylformamide-*O*)(pyridine) platinum(*II*), 10CI

[70347-99-8]



R = H

M 418.1

Probably *trans*-square planar, as shown. Synth. from Di-μ-chlorodichlorobis(pyridine)diplatinum(*II*), IC-006812 + DMF. Yellow solid. Sol. $CHCl_3$. Mp 125°.

Kong, P.-C. *et al*, *Can. J. Chem.*, 1979, **57**, 682 (*synth, ir, pmr*)

$C_8H_{12}Cl_2N_4NiO_8$ IC-005970

Tetrakis(acetonitrile)bis(perchlorato-*O*)nickel(*II*)

Nickel(II) *perchlorate tetrakis(acetonitrile)*

[14058-05-0]

$Ni(OClO_3)_2(NCCH_3)_4$

M 421.8

trans-Octahedral with monodentate $ClO_4^{\ominus}$. Standard reference for ir of monodentate ClO_4. Pale-blue powder; sensitive to H_2O and org. solvs.

▷ Potentially explosive.

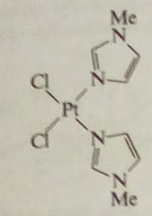
Wickenden, A.E. *et al*, *Inorg. Chem.*, 1965, **4**, 404 (*synth, ir*)

IC-005971

$C_8H_{12}Cl_2N_4Pt$

Dichlorobis(1-methyl-1*H*-imidazole-N^3)platinum(*II*), 9CI

Platinum(II) *chloride bis(1-methylimidazole)*



M 430.1

Forms in 4 cryst. modifications, all with *cis*-square planar configuration. Synth. from Tetrachloroplatinate(*II*)(2−), IC-017117 + $I^{\ominus}$, MeIm, $Ag^{\oplus}$, $Cl^{\ominus}$.

***cis*-form** [61617-01-4]

Appearance not described. Sol. DMF.

***trans*-form** [52585-20-3]

Existence doubtful.

Graves, B.J. *et al*, *Inorg. Chem.*, 1978, **17**, 3007 (*synth, ir, struct*)

$C_8H_{12}Cl_2N_4Ru$ IC-005972

Tetrakis(acetonitrile)dichlororuthenium(*II*), 9CI

Dichlorotetrakis(ethanenitrile)ruthenium(II)

[30066-40-1]

$Ru(N{\equiv}CCH_3)_4Cl_2$

M 336.1

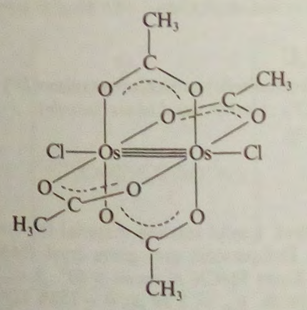
trans-Octahedral. Prepd. by reducing '$RuCl_3.xH_2O$' in MeCN with H_2 (PtO_2 catalyst). Useful synthetic reagent. Yellow solid. Sol. MeCN. Mp 205° dec. Ir ν_{RuCl} 276; ν_{CN} 2270 cm^{-1}.

Gilbert, J.D. *et al*, *J. Chem. Soc. A*, 1970, 2764 (*synth, ir*)
Newton, W.E. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 349 (*synth, ir*)
Inorg. Synth., 1989, **26**, 68 (*reaction*)

$C_8H_{12}Cl_2O_8Os_2$ IC-005973

Tetrakis[μ-(acetato-*O*,*O*′)]dichlorodiosmium(*III*)

[81519-41-7]



M 687.4

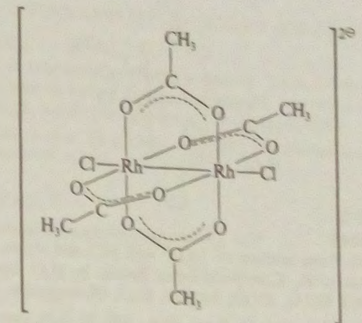
Synth. from $[OsCl_6]^{2\ominus}$ in $AcOH/Ac_2O$. Starting material for many Os—Os bonded compds. Dark red. Insol. org. solvs. Mp 273-275°.

Behling, T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2109 (*synth, ms, ir, uv*)
Fanwick, P.E. *et al*, *Inorg. Chem.*, 1986, **25**, 4546 (*use*)
Tooze, R.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 2711 (*use*)
Cotton, F.A. *et al*, *Polyhedron*, 1986, **5**, 903 (*use*)
Clark, R.J.H. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 5968 (*ir, raman*)
Cotton, F.A. *et al*, *Inorg. Chim. Acta*, 1989, **166**, 109.

$C_8H_{12}Cl_2O_8Rh_2^{2\ominus}$ IC-005974

Tetrakis[μ-(acetato-*O*:*O*′)]dichlorodirhodate(*II*)(2−), 11CI

[71844-86-5]



M 512.8 (ion)

Typical carboxylate-bridged binuclear rhodium struct.

Di-Li salt: [88945-58-8].

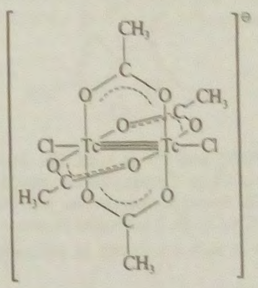
Green cryst. + $8H_2O$.

Miskowski, V.M. *et al*, *Inorg. Chem.*, 1984, **23**, 1154 (*synth, cryst struct, uv*)

$C_8H_{12}Cl_2O_8Tc_2^{\ominus}$ IC-005975

Tetrakis[μ-(acetato-*O*:*O*′)]dichloroditechnetate(1−), 11CI

[82391-75-1]



M 504.8 (ion)

Tc—Tc bond order may be as high as 4 or 4½, though bond order 3½ most favoured. Synth. from $K_3[Tc_2Cl_8]$ + HOAc (autoclave). Can be reduced to uncharged $Tc_2(OAc)_4Cl_2$.

K salt: [78005-19-3].

Tetragonal cryst.

[75846-64-9]

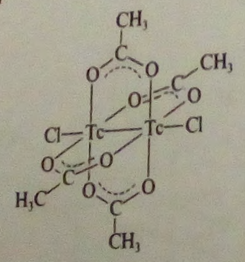
Spitsyn, V.I. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1981, **256**, 608 (*synth, ir, magnetism*)
Nefedev, V.I. *et al*, *Inorg. Chim. Acta*, 1982, **64**, L177 (*bonding*)
Koz'min, P.A. *et al*, *Koord. Khim.*, 1982, **8**, 851 (*cryst struct*)
Rakitin, Yu.V. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1983, **269**, 1123 (*magnetism*)
Rakitin, Yu.V. *et al*, *Zh. Neorg. Khim.*, 1984, **29**, 510; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1984, **29**, 294 (*esr*)

IC-005976

$C_8H_{12}Cl_2O_8Tc_2$

Tetrakis[μ-(acetato-*O*,*O*′)]dichloroditechnetium(*III*)

[75846-64-9]



M 504.8

Synth. from reaction of $TcO_4^{\ominus}$ with HCl and HOAc in an atm. of H_2. Cherry-red cryst., hydrol. by H_2O. Insol. HCl, HOAc, EtOH, Me_2CO, Et_2O. Diamagnetic.

Zaitseva, L.L. *et al*, *Zh. Neorg. Khim.*, 1980, **25**, 2624; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1980, **25**, 1449 (*synth, ir, struct, thermal anal*)

Nefedev, V.I. *et al*, *Inorg. Chim. Acta*, 1982, **64**, L177 (*bonding*)

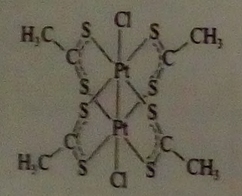
IC-005977

$C_8H_{12}Cl_2Pt_2S_8$

Dichlorotetrakis(dithioacetato)diplatinum(*III*)

Dichlorotetrakis[μ-(ethanedithioato-S,S′)]diplatinum(III), *10CI*

[83897-63-6]



M 825.7

Formally Pt(*III*) with Pt—Pt bond. Obt. by oxidative addition of Cl_2 to Tetrakis(dithioacetato)diplatinum(*II*), IC-006020. Brown microcrystalline solid. Spar. sol. toluene, CH_2Cl_2. Br, I analogues known.

Bellitto, C. *et al*, *Inorg. Chem.*, 1983, **22**, 444 (*synth, ur, pe*)

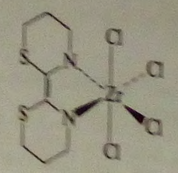
IC-005978

$C_8H_{12}Cl_4N_2S_2Zr$

(2,2′-Bi-2-thiazine)tetrachlorozirconium(*IV*)

Tetrachloro(5,5′,6,6′-tetrahydro-2,2′-bi-4H-1,3-thiazine-N³,N³′)zirconium(IV), *11CI*

[92315-30-5]



M 433.3

The bulk of the ligand is thought to prevent 8-coordination, cf Bis(2,2′-bithiazoline) tetrachlorozirconium(*IV*), IC-007669. Synth. from $ZrCl_4$ and the ligand in 1,2-dichloroethane. White solid. Sol. toluene, MeCN.

Johnson, R.A. *et al*, *Inorg. Chem.*, 1984, **23**, 4302 (*cryst struct, synth, ir*)

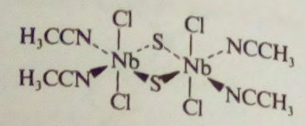
$C_8H_{12}Cl_4N_4Nb_2S_2$

IC-005979

Tetrakis(acetonitrile)tetrachlorodi-μ-thioxodiniobium(*IV*) 10CI

Bis(μ-thio)bis[dichlorobis(methyl cyanide)niobium(IV)]. *Bis(μ-sulfido)bis[dichlorobis(methyl cyanide)niobium*(IV)]

[78420-85-6]



M 555.9

Bioctahedral. Synth. from $NbCl_4(MeCN)_3$ with Sb_2S_3 in MeCN in a sealed ampoule. Brown, v. air-sensitive cryst. + 2MeCN; mono-MeCN solvate also known.

[78391-28-3]

Benton, A.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1304 (*synth, cryst struct*)

IC-005980

$C_8H_{12}Cl_4N_4Pa$

Tetrakis(acetonitrile)tetrachloroprotactinium(*IV*)

$(MeCN)_4PaCl_4$

M 537.0

Moisture-sensitive yellow-green solid. Ir ν_{CN} 2275 cm^{-1}.

Brown, D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 279 (*synth, ir*)

Inorg. Synth., 1970, **12**, 226 (*synth*)

IC-005981

$C_8H_{12}Cl_4N_4Th$

Tetrakis(acetonitrile)tetrachlorothorium(*IV*)

Thorium(IV) *chloride tetrakis(acetonitrile)*

[17499-62-6]

$ThCl_4(MeCN)_4$

M 538.0

Deliquescent colourless cryst. Ir $\nu_{C\equiv N}$ 2273 (2278)cm^{-1}. Loses MeCN *in vacuo* above 40-50°.

Bagnall, K.W. *et al*, *J. Chem. Soc. A*, 1966, 1763 (*synth, ir*)

Feltz, A., *Z. Chem.*, (Leipzig), 1966, **6**, 318.

Inorg. Synth., 1970, **12**, 225 (*synth*)

Kumar, N. *et al*, *Can. J. Chem.*, 1982, **60**, 2597 (*synth, ir*)

IC-005982

$C_8H_{12}Cl_4N_4U$

Tetrakis(acetonitrile)tetrachlorouranium(*IV*)

Uranium(IV) *chloride tetrakis(acetonitrile)*

[17499-63-7]

$(H_3CCN)_4UCl_4$

M 544.0

Dodecahedral. Useful starting material for synth. of UCl_4 compds. Deliquescent grey-green cryst. (MeCN). Sol. MeCN. Loses MeCN *in vacuo* >40°. Ir $\nu_{C\equiv N}$ 2278 cm^{-1}. Paramagnetic, μ_{eff} = 2.89 μ_B; θ −158K (298K).

Bagnall, K.W. *et al*, *J. Chem. Soc. A*, 1966, 1763 (*synth, ir*)

Gans, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 46 (*synth, ur, magnetism*)

Cotton, F.A. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 1186 (*cryst struct*)

Kumar, N. *et al*, *Inorg. Chim. Acta*, 1984, **95**, 211 (*synth, ir*)

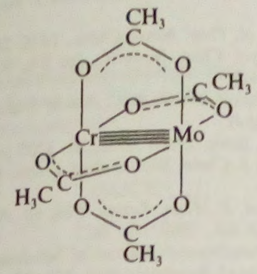
Van den Bossche, G. *et al*, *Acta Crystallogr., Sect. C*, 1989, **45**, 1478 (*cryst struct*)

IC-005983

$C_8H_{12}CrMoO_8$

Tetrakis[μ-(acetato-*O*:*O*′)](chromium)molybdenum, 11CI, 10CI

[54235-41-5]



M 384.1

Quadruple bond easily cleaved; Cr—Mo 205.0 pm. Isomorphous with corresp. Mo_2 compd. Synth. from $Mo(CO)_6$ and $Cr_2(OAc)_4(OH_2)_2$ in $HOAc/Ac_2O/CH_2Cl_2$. First compd. to contain heteronuclear quadruple metal-metal bond. Pale yellow solid (by subl.). Spar. sol. H_2O, $CHCl_3$; sol. Py. $Subl._{0.01}$ 170°.

Garner, C.D. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 3526 (*cryst struct, synth, props*)

Cavell, K.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1714 (*thermochem*)

IC-005984

$C_8H_{12}CrN_4^{2\oplus}$

Tetrakis(acetonitrile)chromium(*II*)(2+), 10CI

Tetrakis(methyl cyanide)chromium(2+)

$[Cr(NCCH_3)_4]^{2\oplus}$

M 216.2 (ion)

Possibly weakly coordinated by $BF_4^{\ominus}$ counterion giving 6-coordinate sp.

Bis-tetrafluoroborate: [76933-11-4].

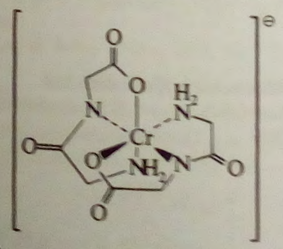
Prep. by electrochemical oxidation. Pink solid. Sol. MeCN; sl. sol. MeOH.

Habeeb, J.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 118 (*synth*)

IC-005985

$C_8H_{12}CrN_4O_6^{\ominus}$

Bis[*N*-glycylglycinato(2−)-*N*,*N*′,*O*²]chromate(*III*)(1−)



M 312.2 (ion)

Cr—N_{amino} 207.9, Cr—$N_{peptide}$ 195.6, Cr—$O_{carboxy}$ 199.1 *mer* config.

Na salt: [105302-05-4].

Synth. from *trans*-tetraaquadichlorochromium(*III*) chloride + ligand in MeOH + NaOH. Monoclinic blue-purple cryst. + $4.5H_2O$ (H_2O). Sol. H_2O.

K salt, complex with 2,5-piperazinediione: [115795-30-7]. Purple cryst. + $2H_2O$. Sol. H_2O.

[115795-29-4]

Murdoch, C.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 1329 (*cryst struct, synth, us-vis*)

Subramanian, V. *et al*, *Polyhedron*, 1988, **7**, 523 (*cryst struct, ir*)

IC-005986

$C_8H_{12}CrO_4S_3$

[[Thiobis(ethylenethio)]diacetato]chromium

[2,2′-[*Thiobis*(2,1-*ethanediylthio*)]*bis*[*acetato*](2−)]*chromium*. (*Diethylenetrithiodiacetato*)*chromium*(II)

$Cr^{2\oplus}[^{\ominus}OOCCH_2SCH_2CH_2SCH_2CH_2SCH_2COO^{\ominus}]$

M 320.3

Obt. as trihydrate; probably polymeric. Synth. from $CrSO_4$ + sodium salt of ligand. Red amorph. powder + $3H_2O$. Antiferromagnetic. $\mu_{eff} \approx 2.05\mu_B$ (298K).

Podlaha, J. *et al*, *Inorg. Chim. Acta*, 1971, **5**, 420 (*synth, uv-vis, magnetism, ir, dta*)

IC-005987

$C_8H_{12}CuN_4^{\oplus}$

Tetrakis(acetonitrile)copper(1+), 9CI

$(H_3CCN)_4Cu^{\oplus}$

M 227.7 (ion)

Hexafluorophosphate:

$C_8H_{12}CuF_6N_4P$ M 372.7

Used for synth. of Cu(I) complexes in nonaqueous media. Cryst. ($MeCN/Et_2O$ at −20°). Mod. sol. polar org. solvs. Air-sensitive as solid.

Maspero, F. *et al*, *J. Organomet. Chem.*, 1972, **38**, C43 (*use*)

Csoregh, I. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 314 (*cryst struct*)

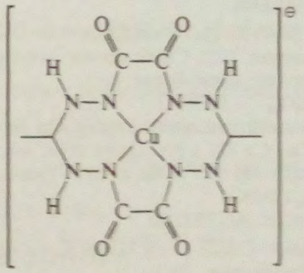
Eller, P.G. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 4346 (*use*)

Inorg. Synth., 1979, **19**, 90 (*synth*)

IC-005988

$C_8H_{12}CuN_8O_4^{\ominus}$

[3,10-Dimethyl-1,2,4,5,8,9,11,12-octaazacyclotetradecane-6,7,13,14-tetronato(4−)-N^1,N^5,N^8,N^{12}]cuprate(*III*)(1−), 11CI



M 347.7 (ion)

Previously thought to contain bonded molecular O_2. Planar anion of Cu(*III*).

Et_3NH salt: [84179-26-0].

Good model for copper oxidase. Deep blue aq. soln., stable for long periods at pH 8-9. Sol. H_2O. Blue intermed. in prepn. of Aqua[7,9,16,18,19,20-hexamethyl-8,17-dioxa-1,2,5,6,10,11,14,15-octaazatricyclo[13.3.1.1^{4,10}]eicosane-3,4,12,13-tetronato(4−)-N^2,N^5,N^{11},N^{14}]cuprate(2−), IC-009402.

Oliver, K.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 1111 (*cryst struct*)

IC-005989

$C_8H_{12}CuO_8^{2\ominus}$

Tetrakis(acetato-*O*)cuprate(*II*)(2−)

$[Cu(OAc)_4]^{2\ominus}$

M 299.7 (ion)

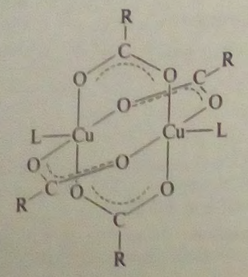
All 8 acetate oxygens interact with Cu, with 4 short (197 pm) and 4 long (279 pm) distances.

Ca salt, hexahydrate: [29012-55-3].
Cryst. Acetate and aqua-bridged chain struct. of alternating Cu and Ca.

Holden, A. *et al, Crystals and Crystal Growing*, Heinemann, London, 1960, 118 (*synth*)
Langs, D.A. *et al, J. Chem. Soc., Chem. Commun.*, 1967, 890 (*cryst struct*)
Klop, E.A. *et al, Acta Crystallogr., Sect. C*, 1983, **39**, 1342 (*cryst struct*)

IC-005990

$C_8H_{12}Cu_2O_8$
Tetrakis[μ-(acetato-*O*:*O*′)]dicopper
Anhydrous cupric acetate
[142-71-2]



dihydrate

R = CH_3
L = OH_2

M 363.2
Usually available as dihydrate. Commercially available. Fungicide, catalyst for organic reactions, ageing of rubber, as pigment for ceramics, in textile dyeing. ^{64}Cu compd. used as radioactive agent.
▷ Toxic. AG3480000.

Dihydrate: [6046-93-1]. *Tetrakis[μ-(acetato-*O*:*O*′)]diaquadicopper, 11Cl. Cupric acetate monohydrate. Copper acetate dimer diaqua*
$C_8H_{16}Cu_2O_{10}$ M 399.3
Contains antiferromagnetic interactions between Cu atoms, Cu—Cu 261.6 pm. Green cryst. Sol. H_2O, EtOH; sl. sol. Et_2O. Mp 115°. Dec. at 240°. Paramagnetic, $\mu_{eff} = 1.40\mu_B$ (293K).
▷ Irritant, toxic. AG3500000.

Bis-Py complex: [15227-71-1]. *Tetrakis[μ-(acetato-*O*:*O*′)]bis(pyridine)dicopper, 11Cl*
$C_{18}H_{22}Cu_2N_2O_8$ M 521.4
Dark green acicular cryst. Insol. EtOH; sol. dioxan. Paramagnetic; $\mu_{eff} = 1.35\mu_B$ (290K). Antiferromagnetic interaction between Cu atoms; Cu—Cu 263.0 pm.
'Monomer': *Copper(II) acetate. Cupric acetate. Crystallised verdigris. Neutral verdigris*
$C_4H_6CuO_4$ M 181.6
Not separately identified.

van Niekerk, J.N. *et al, Acta Crystallogr.*, 1953, **6**, 227 (*cryst struct*)
Figgis, B.N. *et al, J. Chem. Soc.*, 1956, 3837 (*magnetism synth*)
Martin, R.L. *et al, J. Chem. Soc.*, 1957, 2545 (*synth, magnetism*)
Barclay, G.A. *et al, J. Chem. Soc.*, 1961, 5244 (*struct, Py compd*)
van Niekerk, J.N. *et al, Acta Crystallogr.*, 1963, **6**, 227 (*cryst struct*)
Kato, M. *et al, Chem. Rev.*, 1964, **64**, 99 (*rev*)
Kokot, E. *et al, Inorg. Chem.*, 1964, **3**, 1306 (*magnetism, synth, Py compd*)
Kokoszka, G.F. *et al, J. Chem. Phys.*, 1965, **42**, 3693 (*esr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 159; 1969, **2**, 84; 1972, **3**, 65; 1974, **4**, 105; 1975, **5**, 156; 1977, **6**, 138; 1979, **10**, 103; 1980, **12**, 140 (*uses*)

Jotham, R.W. *et al, Inorg. Chem.*, 1970, **9**, 1390 (*magnetism, theory*)
Brown, G.M. *et al, Acta Crystallogr., Sect. B*, 1973, **29**, 2393 (*ntd*)
de Meester, P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2575 (*cryst struct*)
Fletcher, S.R. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2575 (*cryst struct*)
Doedens, R.J. *et al, Prog. Inorg. Chem.*, 1976, **21**, 209 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd Ed., Wiley N.Y., 1978-1984, **6**, 267 (*rev*)
Beddoes, R.L. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 2119 (*synth, Py compd*)
Mathey, Y. *et al, Inorg. Chem.*, 1982, **21**, 3409 (*raman, Py compd*)
Debroy, A. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2531 (*synth, Py compd*)
Hoffmann, S. *et al, J. Magn. Reson.*, 1986, **68**, 490 (*esr, Py compd*)
Merck Index, 11th Ed., 1989, No. 2627.
Sax, N.I. *et al, Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, 950, 951 (*tox*)

$C_8H_{12}GeO_8$ IC-005991
Germanium(*IV*) acetate
Acetic acid, germanium(4+) salt, 9Cl.
Tetraacetoxygermane
[3396-12-1]

$Ge(OAc)_4$

M 308.7
The acetate ligands are unidentate. Fine needles. Easily hydrol. to AcOH and germanic acid. Sol. C_6H_6, Me_2CO. Mp 156°.

Schmidt, H. *et al, Angew. Chem.*, 1947, **59**, 233 (*synth*)
Alcock, N.W. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 2238, 2243 (*synth, ir, pmr, struct*)
Staughan, B.P. *et al, Spectrochim. Acta, Part A*, 1986, **42**, 451 (*ir, raman, pmr, cmr*)

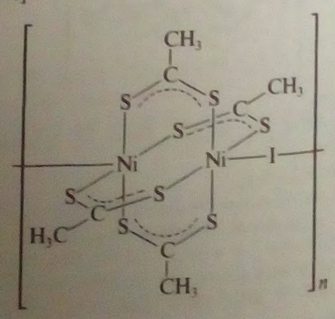
$C_8H_{12}HgN_4^{2\oplus}$ IC-005992
Tetrakis(acetonitrile)mercury(2+)

$[Hg(NCCH_3)_4]^{2\oplus}$

M 364.8 (ion)
Bis-hexafluoromolybdate(1−): [56841-13-5].
$C_8H_{12}F_{12}HgMo_2N_4$ M 784.6
Cryst.

Prescott, A. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 936 (*synth*)

$C_8H_{12}INi_2S_8$ IC-005993
Tetrakis[μ-(dithioacetato)]iododinickel
Tetrakis[μ-[ethane(dithioato)-S:S′]]iododinickel, 11Cl
[95974-44-0]



M 608.9

Diamagnetic semiconductor (Hopping-electron conductor). Iodine atoms bridge dimeric units. Black needles (CS_2). Sl. sol. CS_2. Dec. > 126°.

Bellitto, C. *et al, Inorg. Chem.*, 1985, **24**, 2815 (*synth, cryst struct, ir, uv-vis, pe*)

$C_8H_{12}I_4N_4U$ IC-005994
Tetrakis(acetonitrile)tetraiodouranium(*IV*)
Tetraiodotetrakis(methyl cyanide)uranium(IV). *Uranium*(IV) *iodide tetrakis(acetonitrile)*
[105331-71-3]

$(MeCN)_4UI_4$

M 909.8
Starting material for other UI_4 complexes. Hygroscopic orange-red cryst. (MeCN). Cannot be desolvated without dec. Dec. with loss of MeCN > 50°.

du Preez, J.G.H. *et al, Inorg. Chim. Acta*, 1986, **118**, 225.
du Preez, J.G.H. *et al, J. Chem. Soc., Chem. Commun.*, 1986, 743 (*synth*)

$C_8H_{12}IrN_4^{\oplus}$ IC-005995
Tetrakis(isocyanomethane)iridium(1+), 9Cl
Tetrakis(methylisonitrile)iridium(1+). Tetrakis(methyl isocyanide)iridium(1+)

$[Ir(CNMe)_4]^{\oplus}$

M 356.4 (ion)
Chloride: [40226-52-6].
$C_8H_{12}ClIrN_4$ M 391.8
Air-sensitive blue-black cryst.
Iodide: [40226-55-9].
$C_8H_{12}IIrN_4$ M 483.3
Air-sensitive cryst.
Hexafluorophosphate: [40226-53-7].
$C_8H_{12}F_6IrN_4P$ M 501.3
Air-sensitive cryst.
Perchlorate: [40226-64-0].
$C_8H_{12}ClIrN_4O_4$ M 455.8
Air-sensitive cryst.
Tetraphenylborate: [40226-54-8].
$C_{32}H_{32}BIrN_4$ M 675.6
Air-sensitive cryst.

Bedford, W.M. *et al, J. Chem. Soc., Chem. Commun.*, 1972, 1224 (*synth, ir, pmr*)
Geoffrey, G.L. *et al, Inorg. Chem.*, 1978, **17**, 777 (*synth*)

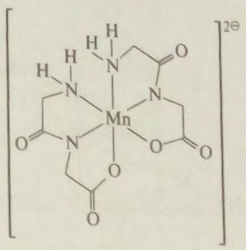
$C_8H_{12}MnN_4^{2\oplus}$ IC-005996
Tetrakis(acetonitrile)manganese(2+), 11Cl
Tetrakis(methyl cyanide)manganese(2+)

$[Mn(NCCH_3)_4]^{2\oplus}$

M 219.1 (ion)
Counter anion weakly bound to give *trans*-octahedral molecules in solid state. Synth. from a suspension of NOX (X = BF_4, ClO_4) and Mn metal in MeCN.
Bis-tetrafluoroborate:
$C_8H_{12}B_2F_8MnN_4$ M 392.7
White cryst. (MeCN/EtOAc). Mp 110-111°. $\mu_{eff} = 5.90\mu_B$.
Diperchlorate: [94859-45-7]. *Manganese*(II) *perchlorate tetrakis(acetonitrile)*
$C_8H_{12}Cl_2MnN_4O_8$ M 418.0
▷ Potentially explosive.

Hathaway, B.J. *et al, J. Chem. Soc.*, 1961, 3091 (*synth, ir*)
Hathaway, B.J. *et al, J. Chem. Soc.*, 1962, 2444 (*synth, ir, magnetism, dta, tga*)
Reedijk, J. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1968, **87**, 1079 (*ir, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 9 (*rev, bibl*)

$C_8H_{12}MnN_4O_6^{2\ominus}$ IC-005997
Bis[*N*-glycylglycinato(2−)-*N*,N^N,O^1]manganate(*II*)(2−), 10Cl



M 315.1 (ion)
Octahedral, precise struct. not known.
Di-Na salt: [62793-12-8].
Prepd. from glycylglycine in EtOH and freshly prepared $Mn(OH)_2$ in aq. NaOH. Cryst. $+2H_2O$.

Hodgson, J.B. *et al, J. Mol. Struct.*, 1977, **37**, 193 (*synth, ir, struct*)
Kittl, W.S. *et al, Inorg. Chim. Acta*, 1982, **63**, 47 (*stability const*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 340 (*rev, bibl*)

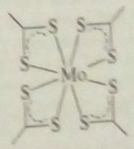
$C_8H_{12}MnO_8^{2\ominus}$ IC-005998
Tetrakis(acetato-*O*)manganate(*II*)(2−)
Tetra(acetato)manganate(II)(2−)

$[Mn(OAc)_4]^{2\ominus}$

M 291.1 (ion)
Struct. not known. Synth. from alkali metal acetate and $Mn(OAc)_2$ in EtOH.
Di-Na salt: [67414-37-3].
Solid + H_2O. Sol. H_2O, MeOH, EtOH; insol. C_6H_6, pet. ether, CCl_4.
Di-K salt: [67414-38-4].
Solid + H_2O. Soly. as for Na salt.
Di-NH_4 salt: [67414-39-5].
Solid + H_2O.

Kharitonov, Yu.Ya. *et al, Koord. Khim.*, 1978, **4**, 946 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 52 (*rev, bibl*)

$C_8H_{12}MoS_8$ IC-005999
Tetrakis(dithioacetato)molybdenum(*IV*)
Tetrakis[ethane(dithioato)-S,S′]molybdenum, 10Cl.
Molybdenum(IV) *dithioacetate*
[68340-66-9]



M 460.6
8-Coordinate triangular dodecahedron. Used as host for V(*IV*) and Nb(*IV*) in esr studies. Cryst. V. sol. CS_2, toluene. Diamagnetic.

Dessy, G. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3066 (*cryst struct*)
Attanasio, D. *et al*, *Inorg. Chem.*, 1980, **19**, 3419 (*use*)

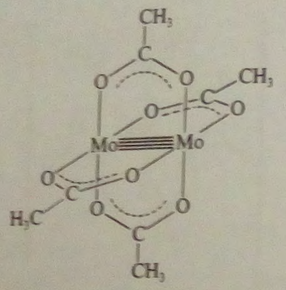
IC-006000

$C_8H_{12}Mo_2O_8$

Tetrakis[μ-(acetato-*O*:*O*′)]dimolybdenum(*II*), 10Cl, 9Cl, 8Cl

Dimolybdenum tetraacetate

[14221-06-8]



M 428.0
Synth. from $Mo(CO)_6$ + AcOH + Ac_2O. Precursor to Mo≡Mo compds. Catalyses ring opening polym. Yellow, air-sensitive cryst. (diglyme). Spar. sol. polar org. solvs; insol. non-polar solvs. Subl. 300° *in vacuo*.

Monomer: [11071-39-9]. *Molybdenum*(II) *acetate*
$C_4H_4MoO_4$ M 214.0
Has no separate existence.

Stephenson, T.A. *et al*, *J. Chem. Soc.*, 1964, 2538 (*synth, ir, props*)
Lawton, D. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 921 (*cryst struct*)
Inorg. Synth., 1971, **13**, 81 (*synth, props*)
Cotton, F.A. *et al*, *Acta Crystallogr., Sect. B*, 1974, **30**, 2768 (*cryst struct*)
Smith, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 1742 (*use*)
Hino, K. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 2164 (*cryst struct*)
Greaves, R.A. *et al*, *Polyhedron*, 1986, **5**, 415 (*Mo-95 nmr*)

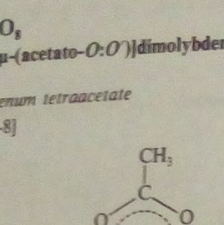
IC-006001

$C_8H_{12}N_2O_2RuS_4$

Dicarbonylbis(*N*,*N*-dimethyldithiocarbamato)ruthenium(*II*)

Dicarbonylbis(dimethylcarbamodithioato-S,S′)ruthenium, 9Cl

[15393-11-0]



M 397.5
Prepd. by treating the red soln. obt. by passing CO through ethanolic $RuCl_3.xH_2O$, or $[Ru_3(CO)_{12}]$, with $Me_2NCS_2CS_2NMe_2$. Yellow cryst. (EtOH). Sol. CH_2Cl_2. Mp 230-231°. Subl. 170°. Ir ν_{CO} 2020, 1901 cm^{-1} (CH_2Cl_2).

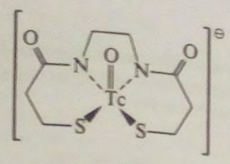
Kingston, J.V. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 2709 (*synth, ir*)
Cole-Hamilton, D.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 739 (*synth, pmr*)

IC-006002

$C_8H_{12}N_2O_3S_2Tc^{\ominus}$

[[*N*,*N*′-1,2-Ethanediylbis[3-mercaptopropanamidato]](4−)-*N*,*N*′,*S*,*S*′]oxotechnetate(*V*)(1−), 10Cl

Oxo[N,N′-*ethylenebis*(*3-mercaptopropionimidato*)]*technetate*(V)



M 347.2 (ion)
Synth. from $TcO_4^{\ominus}$ + H_4L with dithionite reduction.

Ph_4As salt: [75961-54-5].
Orange cryst. (Me_2CO aq.). Mp 187-189°.

Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 1629 (*synth, str, ir, pmr*)

IC-006003

$C_8H_{12}N_4Pd^{2\ominus}$

Tetrakis(acetonitrile)palladium(2+), 8Cl

Tetrakis(methyl cyanide)palladium(2+)

$[Pd(NCCH_3)_4]^{2\ominus}$ (D_{4h})

M 270.6 (ion)

Bis-tetrafluoroborate: [21797-13-7].
Catalyses polym. of styrene. Yellow cryst. ($MeCN/Et_2O$).

Bis-trifluoromethanesulfonate: [68569-14-2].
Catalyses prepn. of unsaturated amines. No physical data available.

Bis-hexachloroantimonate: [17500-34-4].
No physical data available.

Bis-tetrachlorothallate: [21374-01-6].
Mp 83-86° dec.

Reedijk, J. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1967, **86**, 1127; 1968, **87**, 513 (*ir, synth*)
Schrann, R.F. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 898 (*synth, ir*)
Sen, A. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4627 (*use*)
Hegedus, L.S. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 6224 (*use*)

IC-006004

$C_8H_{12}N_4Pt^{2\ominus}$

Tetrakis(isocyanomethane)platinum(*II*)(2+), 9Cl

Tetrakis(methyl isonitrile)platinum(II)(2+)

[45073-89-0]

$[Pt(CNMe)_4]^{2\ominus}$ (D_{4h})

M 359.2 (ion)

Bis-hexafluorophosphate: [38317-61-2].
Cryst. (MeCN). Ir ν_{CN} 2308 cm^{-1}.

Bis-tetrafluoroborate: [33989-89-8].
Cryst. (MeCN/EtOAc). Mp 224-227°. Ir ν_{CN} 2300 cm^{-1}.

Tetrakis(cyano-C)platinate(2−): [50600-86-7].
$C_{12}H_{12}N_8Pt_2$ M 658.4
Bright yellow fluorescent cryst. (CH_2Cl_2).

Treichel, P.M. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 5424 (*synth, ir, pmr*)
Miller, J.S. *et al*, *Inorg. Chem.*, 1972, **11**, 2069 (*synth, ir, pmr*)
Isci, H. *et al*, *Inorg. Chem.*, 1974, **13**, 1175; 1975, **14**, 913 (*synth, ir, pmr, str*)

IC-006005

$C_8H_{12}N_4Zn^{2\ominus}$

Tetrakis(acetonitrile)zinc(2+)

$[Zn(N{\equiv}CCH_3)_4]^{2\ominus}$

M 229.6 (ion)

Bisulfate: [58079-29-1].
$C_8H_{14}N_4O_8S_2Zn$ M 423.7
Loses MeCN at atmospheric pressure.

Bis-fluorosulfate: [25753-49-5]. *Zinc*(II) *fluorosulfate tetrakis(acetonitrile)*
Synth. from $Zn(FSO_3)_2$ in MeCN. Cryst.

Milne, J.B., *Can. J. Chem.*, 1970, **48**, 75 (*synth, ir, props*)
Crookes, J.V. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 2060 (*synth*)

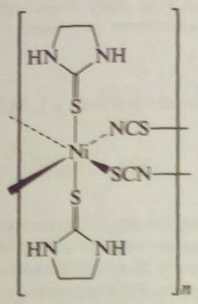
IC-006006

$C_8H_{12}N_8NiS_4$

Bis(2-imidazolidinethione-*S*)bis(thiocyanato-*N*)nickel(*II*), 9Cl

Bis(2-thioimidazolidine)bis(thiocyanato)nickel(II).
Bis(ethylenethiourea)bis(thiocyanato)nickel(II)

[14973-25-2]



M 379.1
Chain struct. with octahedral Ni and bridging NCS groups. Green cryst. (EtOH aq.). Sol. H_2O, EtOH, MeOH. μ_{eff} = 3.11μ_B (293K). Exhibits antiferromagnetic coupling between neighbouring ferromagnetic chains.

[35232-21-4]

Nardelli, M. *et al*, *Acta Crystallogr.*, 1966, **21**, 910 (*synth, cryst struct*)
Puglisi, C. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1069 (*synth, uv-vis, magnetism*)
Emori, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 3299 (*magnetism*)

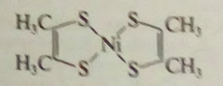
IC-006007

$C_8H_{12}NiS_4$

Bis[2-butene-2,3-dithiolato(2−)-*S*,*S*′]nickel, 9Cl

Dithiobiacetylnickel(II)

[19141-54-9]



M 295.1
Singlet oxygen quencher. Air-stable intensely blue-violet cryst. Mp 256° dec.

[14263-96-8, 38951-94-9]

Schrauzer, G.N. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1964, **3**, 381 (*synth*)
Schrauzer, G.N. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 1483; 1966, **88**, 5174 (*synth, ir, electrochem*)
Zweig, A. *et al*, *J. Polym. Sci., Polym. Chem. Ed.*, 1975, **13**, 717 (*synth, use*)
Siiman, O., *Inorg. Chem.*, 1980, **19**, 2889 (*ir*)
Ahmad, M.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 165 (*synth, str, props*)

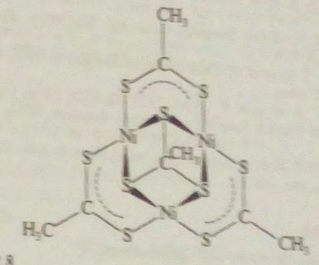
IC-006008

$C_8H_{12}Ni_2S_9$

Tris(dithioacetato)(trithioorthoacetato)trinickel(*II*)

Tris[μ-[*ethane*(*dithioato*)-*S*:*S*′][μ$_3$-[1,1,1-*ethanetrithiolato*(3−)-*S*,*S*′:*S*,*S*′:*S*,*S*′][*trinickel*, 9Cl

[51637-43-5]



M 572.8
Cryst. in two forms. Air-stable shiny-black orthorhombic prisms.

Bonamico, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 2594 (*synth, cryst struct*)

IC-006009

$C_8H_{12}O_4S_4Sn$

Tetrakis(thioacetato)tin

Tin(IV) *monothioacetate*

[76891-08-2]

$Sn(SCOCH_3)_4$

M 419.1
Fine cryst. solid. Sol. common org. solvs.

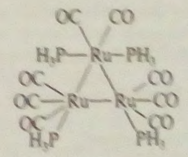
Mehrotra, R.C. *et al*, *Inorg. Chim. Acta*, 1981, **47**, 125 (*synth, ir, pmr*)

IC-006010

$C_8H_{12}O_8P_4Ru_3$

Octacarbonyltetrakis(phosphine)triruthenium, 9Cl

[12347-81-8]



Presumed struct.

M 663.2
No spectroscopic, structural or phys. props. reported.
Synth. by the reaction of PH_3 with $[Ru(CO)_2Cl_2]_n$.

Klanberg, F. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 3296 (*synth*)

IC-006011

$C_8H_{12}O_8Pb$

Lead tetraacetate

Tetrakis(acetato)lead, 8Cl. Lead(IV) *acetate*

[546-67-8]

$Pb(OAc)_4$

M 443.3
Reagent for plumbylation of aromatic compds. and for organic oxidations and related reactions. Colourless prisms; unstable in air. Sol. dry $CHCl_3$, CCl_4, C_6H_6. Sl. sol. AcOH. Dec. by H_2O,alcohols. Mp 175-180°. Dissolves in conc. halogen acids forming haloplumbic acids.

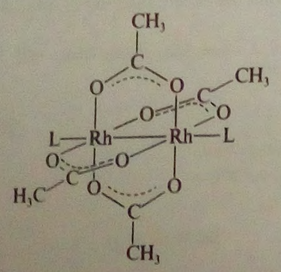
Inorg. Synth., 1939, **1**, 47 (*synth*)

Williams, K.C., *J. Org. Chem.*, 1967, **32**, 4062.
Müller, R. *et al*, *Chem. Ber.*, 1968, **101**, 783.
Willemsens, L.C. *et al*, *J. Organomet. Chem.*, 1968, **13**, 357.
Kamenov, B. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 321 (*cryst struct*)
Syutkina, O.P. *et al*, *Zh. Obshch. Khim.*, 1973, **43**, 1322.
Alcock, N.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2238 (*synth*)
Butler, R.N., *Synth. Reagents*, Pizey, J.S., Ed., Wiley, Chichester, 1977, **3**, 278.
Mitchell, T.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 960 (*cmr, Pb-207 nmr*)
Bell, H.C. *et al*, *Aust. J. Chem.*, 1979, **32**, 1521, 1531.
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1982, **10**, 228.
Straughan, B.P. *et al*, *Spectrochim. Acta, Part A*, 1986, **42**, 451 (*ir, raman, pmr, cmr*)

$C_8H_{12}O_8Rh_2$ IC-006012

Tetrakis[μ-(acetato-*O*:*O*′)]dirhodium(*II*)

Rhodium(II) *acetate dimer*



L = positions of donor ligands

M 441.9

Always obt. as adducts with 2 donor ligands. Synth. e.g. by heating NaOAc + $RhCl_3.3H_2O$ in MeOH.

Dihydrate: [28410-96-0]. *Diaquatetrakis[μ-(acetato-O:O′)]dirhodium*(II), *8CI. Rhodium*(II)*acetate hydrate*
$C_8H_{16}O_{10}Rh_2$ M 478.0
Blue-green cryst.

Dinitrosyl complex: Tetrakis[μ-(acetato-O:O′)]dinitrosyldirhodium
$C_8H_{12}N_2O_{10}Rh_2$ M 502.0
Dark brown solid.

Bis-MeOH complex: [41772-64-9].
$C_{10}H_{20}O_{10}Rh_2$ M 506.0
Blue-green solid. Spar. sol. toluene.

Bis-Et_2NH complex: [69102-54-1].
$C_{16}H_{34}N_2O_8Rh_2$ M 588.2
Dark red needles. Sol. cyclohexane, C_6H_6, toluene with loss of $NHEt_2$.

Bis-tetrahydrothiophene complex: [72207-18-2].
$C_{16}H_{28}O_8Rh_2S_2$ M 618.3
Dark red cryst.

Bis-Py complex: Tetrakis[μ-(acetato-O:O′)]bispyridinedirhodium
$C_{18}H_{22}N_2O_8Rh_2$ M 600.1

Bis-DMSO complex: [39773-10-9]. *Tetrakis[μ-(acetato-O:O′)]bis[sulfinylbis[methane]-S]dirhodium, 10CI. Tetraacetatobis(dimethylsulfoxide)dirhodium*(II)
$C_{12}H_{24}O_{10}Rh_2S_2$ M 598.2
Orange cryst. DMSO ligand coordinates through S.

Bis(isocyanomethane)complex: [80419-75-6].
$C_{12}H_{18}N_2O_8Rh_2$ M 524.0
Dimeric with Rh—Rh bond.

4-Cyanopyridine complex: [73545-75-2]. *Tetrakis[μ-(acetato-O:O′)](4-pyridinecarbonitrile-N′)dirhodium*(III), *10CI*
$C_{14}H_{16}N_2O_8Rh_2$ M 546.1
Synth. from $Rh_2(OAc)_4$(4-cyanopyridine)$_2$ at 150°.
Props. not recorded.

Monomer: Rhodium(II) *acetate*
$C_4H_6O_4Rh$ M 220.9
Has no separate existence.

[29998-99-0]

Johnson, S.A. *et al*, *Inorg. Chem.*, 1963, **2**, 960 (*synth, ir, bis-NO complex*)
Cotton, F.A. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 2926.
Cotton, F.A. *et al*, *Acta Crystallogr., Sect. B*, 1971, **27**, 1664 (*synth, cryst struct, diaqua complex*)
Inorg. Synth., 1972, **13**, 90 (*synth*)
Koh, Y.B. *et al*, *Inorg. Chem.*, 1979, **18**, 1122 (*synth, cryst struct, bis-$NHEt_2$ complex*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1980, **19**, 323 (*synth, cryst struct, bis-tetrahydrothiophene complex*)
Dennis, A.M. *et al*, *Inorg. Chim. Acta*, 1980, **44**, 2139 (*synth, pe, cyano pyridine complex*)
Felthouse, T.R. *et al*, *Prog. Inorg. Chem.*, 1982, **29**, 73 (*synth, bis-MeOH, bis isocyanomethane complexes*)

$C_8H_{12}O_8Rh_2^{\oplus}$ IC-006013

Tetrakis(μ-acetato)dirhodium(1+), 9CI

[15956-28-2]

$[Rh_2(OAc)_4]^{\oplus}$

M 441.9 (ion)

Mixed valence Rh(*II*)—Rh(*III*) carboxylate. Salts not isol. Cation is orange or violet in colour depending on the medium and slowly disproportionates into $Rh_2(OAc)_4$ and Rh(*III*) species. Paramagnetic.

Wilson, C.R. *et al*, *Inorg. Chem.*, 1975, **14**, 2276 (*synth, magnetism, uv, electrochem*)
Cannon, R.D. *et al*, *Inorg. Chem.*, 1981, **20**, 1470 (*synth, kinetics*)

$C_8H_{12}O_8Si$ IC-006014

Silicon(*IV*) acetate

Tetraacetoxysilane. Silicon tetraacetate. Acetic acid, tetraanhydride with silicic acid (H_4SiO_4), 9CI

[562-90-3]

$Si(OAc)_4$

M 264.2

Contains only unidentate acetate. Synth. from $SiCl_4$ + Ac_2O or NaOAc. Hygroscopic cryst. (Ac_2O). Mod. sol. Me_2CO, C_6H_6. Mp 110°.

Inorg. Synth., 1953, **4**, 45 (*synth*)
Udovenko, V.V. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1957, **27**, 985 (*synth*)
Hunter, B.K. *et al*, *Can. J. Chem.*, 1968, **46**, 1399 (*Si-29 nmr*)
Kamenar, B. *et al*, *Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1975, **141**, 97 (*cryst struct*)
Dube, G. *et al*, *Collect. Czech. Chem. Commun.*, 1977, **42**, 2898 (*ms*)
Straughan, B.P. *et al*, *Spectrochim. Acta, Part A*, 1986, **42**, 451 (*ir, raman, struct*)

$C_8H_{12}O_8Sn$ IC-006015

Tetrakis(acetato-*O*,*O*′)tin, 10CI

Tin(IV) *acetate. Tin tetraacetate. Tetraacetoxytin. Tetraacetoxystannane. Acetic acid, tin(4+) salt (4:1)*

[69475-44-1]

$Sn(OAc)_4$

M 354.8

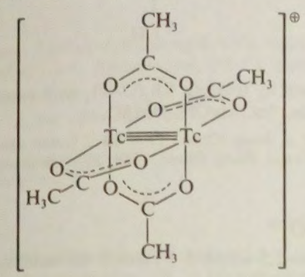
Synth. e.g. from Sn + $Cu(OAc)_2$ in Ac_2O or from $SnPh_4$ in HOAc. White hygroscopic needles (AcOH/Ac_2O). Mp 227-228°.

[2800-96-6]
Rosenberg, S.D. *et al*, *J. Am. Chem. Soc.*, 1955, **79**, 2138 (*synth*)
Garner, C.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 562 (*synth*)
Alcock, N.W. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 80 (*cryst struct*)
Morton, J.R. *et al*, *J. Phys. Chem.*, 1979, **83**, 853.
Wakeshima, I. *et al*, *Chem. Lett.*, 1985, 395 (*synth*)
Blunden, S.J. *et al*, *Inorg. Chim. Acta*, 1986, **116**, L31 (*mössbauer,Sn-119 nmr*)
Straughan, B.P. *et al*, *Spectrochim. Acta, Part A*, 1986, **42**, 451 (*ir, raman*)
Sawyer, A.K. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1989, **19**, 969 (*synth*)

$C_8H_{12}O_8Tc_2^{\oplus}$ IC-006016

Tetrakis(μ-acetato)ditechnetium(1+)

Tetraacetatoditechnetium(1+)



M 433.9 (ion)

Tc—Tc bond order is 3½ (or possibly higher).

Chloride: [78005-18-2]. *Tetrakis[μ-(acetato-O:O′)]chloroditechnetium*
$C_8H_{12}ClO_8Tc_2$ M 469.4
Cryst.

Koz'min, P.A. *et al*, *Koord. Khim.*, 1981, **7**, 1719 (*cryst struct*)
Gerasimov, V.N. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1982, **266**, 148 (*pe*)
Nefedov, V.I. *et al*, *Inorg. Chim. Acta*, 1982, **64**, L177 (*bonding*)
Rakitin, Yu.V. *et al*, *Zh. Neorg. Khim.*, 1984, **29**, 510; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1984, **29**, 294 (*esr*)

$C_8H_{12}O_8U$ IC-006017

Uranium(*IV*) acetate

Tetrakis(*acetato*)*uranium*(IV)

$U(OAc)_4$

M 474.2

Polymeric struct. with 10-coord. U (bicapped square antiprism). Isostructural with Th analogue. Hygroscopic sl. air-sensitive light green solid or monoclinic green cryst. Insol. EtOH, C_6H_6, Et_2O; sl. sol. AcOH. Dec. by hot H_2O. Dec. at *ca* 320°.

Rosenheim, A. *et al*, *Z. Anorg. Allg. Chem.*, 1932, **206**, 33 (*synth*)
Jelenić, I. *et al*, *Acta Crystallogr.*, 1964, **17**, 758 (*cryst struct*)
Selbin, J. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1385 (*synth, uv-vis*)
Inorg. Synth., 1967, **9**, 41.
Eliseev, A.A. *et al*, *Zh. Neorg. Khim.*, 1967, **12**, 2854; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1967, **12**, 1507 (*cryst struct*)
Zhirov, A.I. *et al*, *Radiokhimiya*, 1976, **18**, 644 (*complexes*)

$C_8H_{12}O_8Zn^{2\ominus}$ IC-006018

Tetrakis(acetato-*O*)zincate(2−)

[57088-83-2]

$[Zn(OAc)_4]^{2\ominus}$

M 301.5 (ion)

Di-Na salt: [41743-15-1].
Cryst. Mp 124° dec.

Di-Cs salt: [71817-87-3].
Cryst.

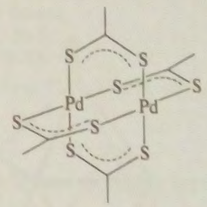
Lehrman, A. *et al*, *J. Am. Chem. Soc.*, 1939, **61**, 3340 (*synth, Na salt*)
Sawada, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2282 (*stability const*)
Kuznetsov, Yu.M. *et al*, *Deposited Doc.*, VINITI, 1978, 1816-78; *CA*, 1979, **91**, 182183 (*cryst struct*)

$C_8H_{12}Pd_2S_8$ IC-006019

Tetrakis(dithioacetato)dipalladium(*II*)

Tetrakis[μ-(ethanedithioato-S,S′)]dipalladium, 10CI. Palladium(II) *dithioacetate dimer*

[63890-11-9]



M 577.5

Struct. not determined, but presumed in light of structs. of derivs. Probably has infinite stack of dimers. Obt. by subl. of either deriv. Red microcrystalline solid. Sl. sol. C_6H_6, $CHCl_3$, CH_2Cl_2.

CS_2 solvate (2:1): [63890-13-1].
Green tetragonal cryst.; turns red with loss of CS_2 in open air. Sl. sol. C_6H_6, $CHCl_3$, CH_2Cl_2. Struct. is stack of dimers with CS_2 between columns.

Compd. with bis(dithioacetato)palladium(II). [63890-12-0]. Synth. from Tetrachloropalladate(*II*)(2−), IC-017115 + CH_3CS_2H. Brick-red monoclinic cryst. Sl. sol. C_6H_6, $CHCl_3$, CH_2Cl_2. Struct. is stack of alternate monomers and dimers. Monomeric and dimeric molecules also coexist in soln. and in the vapour.

Monomer: [63890-10-8]. *Bis(dithioacetato)palladium*(II). *Bis[ethane(dithioato)-S,S′]palladium, 9CI*
$C_4H_6PdS_4$ M 288.7
Synth. from K_2PdCl_4 + CH_3CS_2H. Not obtained separately from the dimer.

[63882-63-3, 70072-39-8, 70072-41-2]

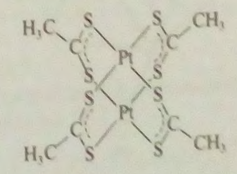
Piovesana, O. *et al*, *Inorg. Chem.*, 1979, **18**, 2258 (*synth, struct, ir, uv, pmr, ms*)

$C_8H_{12}Pt_2S_8$ IC-006020

Tetrakis(dithioacetato)diplatinum(*II*)

Tetrakis[μ-(ethanedithioato-S:S′)]diplatinum(II), *10CI*

[74868-86-3]



M 754.8

Weak inter-dimer Pt—Pt interactions. Undergoes oxidative addition to e.g. Dichlorotetrakis(dithioacetato) diplatinum(*III*), IC-005977. Synth. from $PtCl_4^{2\ominus}$ + CH_3CS_2H. Deep purple needles with red lustre. Sol. C_6H_6, toluene.

Monomer: [74854-48-1]. *Bis(dithioacetato)platinum*(II)
$C_4H_6PtS_4$ M 377.4
Has no separate existence, unlike Pd analogue.

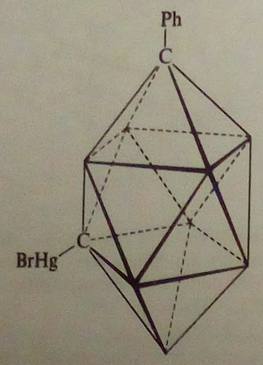
Bellitto, C. *et al, Inorg. Chem.*, 1980, **19**, 3632 (*synth, struct, ir, uv, pmr*)
Bellitto, C. *et al, J. Chem. Soc., Chem. Commun.*, 1981, 409 (*uv*)

$C_8H_{13}B_8BrHg$ IC-006021

Bromo(1-phenyl-1,6-dicarbadecaboran(10)-6-yl)mercury, 9CI

1-Phenyl-6-bromomercuri-1,6-dicarba-closo-*decaborane(10)*

[42570-23-0]



M 476.1
closo-. Sublimable cryst. (heptane). Mp 195-196°.

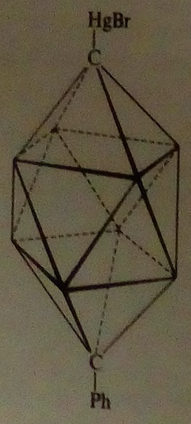
Zakharkin, L.I. *et al, J. Gen. Chem. USSR (Engl. Transl.)*, 1973, **43**, 848 (*synth*)

$C_8H_{13}B_8BrHg$ IC-006022

Bromo(10-phenyl-1,10-dicarbadecaboran(10)-1-yl) mercury, 9CI

1-Phenyl-10-bromomercuri-1,10-dicarba-closo-*decaborane(10)*

[42570-30-9]



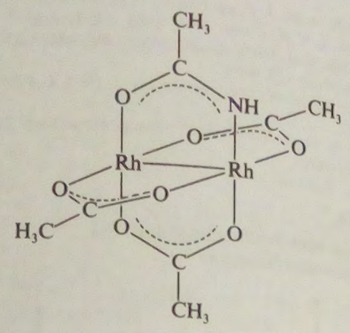
M 476.1
Sublimable cryst. (heptane). Mp 261-262°.

Zakharkin, L.I. *et al, J. Gen. Chem. USSR (Engl. Transl.)*, 1973, **43**, 848 (*synth*)

$C_8H_{13}NO_7Rh_2$ IC-006023

[μ-(Acetamidato-*N*:*O*)]tris[μ-(acetato-*O*:*O'*)] dirhodium(*II*), 11CI

[87985-37-3]



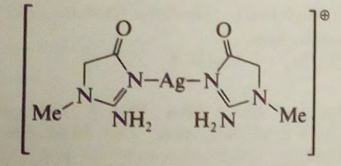
M 441.0
Prepd. *in situ* by treating $Rh_2(OAc)_4$ with excess molten acetamide. Sol. MeCN, DMSO.

Zhu, T.P. *et al, Inorg. Chem.*, 1984, **23**, 2 (*synth, electrochem*)
Chavan, M. *et al, Inorg. Chem.*, 1984, **23**, 4538 (*electrochem, uv, esr*)

$C_8H_{14}AgN_6O_2^{\oplus}$ IC-006024

Bis(2-amino-1,5-dihydro-1-methyl-4*H*-imidazol-4-one-N^3) silver(1+), 10CI

Bis(creatinine)silver(I)(*1+*)



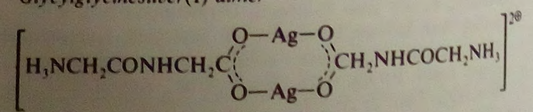
M 334.1 (ion)
Perchlorate: [78713-93-6].
Colourless cryst. + $2H_2O$, light sensitive. Insol. Et_2O.
▷ Potentially explosive.

Udupa, M.R. *et al, Inorg. Chim. Acta*, 1981, **55**, 153 (*cryst struct, synth*)

$C_8H_{16}Ag_2N_4O_6^{2\oplus}$ IC-006025

Bis[μ-(*N*-glycylglycine)]disilver(2+), 8Cl

Glycylglycinesilver(I) *dimer*



M 477.9
8-Membered ring. Model for metal protein interaction.
Dinitrate: [34431-09-9].
Cryst.

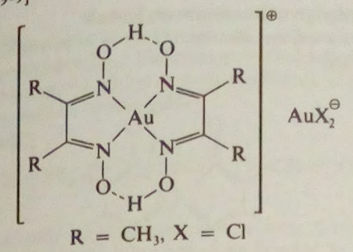
Acland, C.B. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 1017 (*cryst struct, synth*)

$C_8H_{14}Au_2Cl_2N_4O_4$ IC-006026

Bis(dimethylglyoximato)gold(*I*)(1+) dichloroaurate(1−)

Bis[(2,3-butanedione dioximato)(1−)-N,N']gold(1+) dichloroaurate(1−), 9CI

[60105-99-9]



R = CH_3, X = Cl

M 695.0
Mixed valence Au(*I*)Au(*III*) compd. with short intergold contact of 326 pm. Amber cryst. (H_2O); stable to strong acid.

Rundle, R.E., *J. Am. Chem. Soc.*, 1954, **76**, 3101 (*synth, cryst struct*)
Hara, Y. *et al, Solid State Commun.*, 1976, **19**, 171 (*solid state conductivity props*)

$C_8H_{14}BN$ IC-006027

(*N,N*-Dimethylaniline)trihydroboron

Borane N,N-*dimethylaniline*. (N,N-*Dimethylbenzenamine*) *trihydroboron, 10CI*. N,N-*Dimethylbenzenamine compd. with borane(1:1), 9CI*. N,N-*Dimethylaniline compd. with borine*

[1769-74-0]

$PhNMe_2—BH_3$

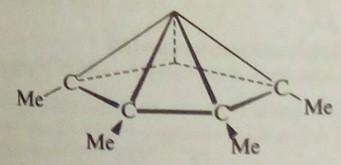
M 135.0
Tested as rocket fuel.

Mikheeva, V.I. *et al, Zh. Neorg. Khim.*, 1957, **2**, 604.
U.K. Pat., 889 599, (1962); *CA*, **61**, P9198d.
Fr. Pat., 1 350 849, (1964); *CA*, **60**, P14327f.
Ashby, E.C., *J. Organomet. Chem.*, 1965, **3**, 371.
Beachley, O.T. *et al, Inorg. Chem.*, 1973, **12**, 1128.

$C_8H_{14}B_2$ IC-006028

2,3,4,5-Tetramethyl-2,3,4,5-tetracarbahexaborane(6), 11CI, 10CI

[71515-14-5]



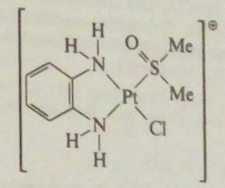
M 131.8
nido-. Sol. $CHCl_3$.

Berger, H.O. *et al, Chem. Ber.*, 1979, **112**, 2884 (*synth, pmr, cmr, B-11 nmr*)
Wrackmeyer, B., *Z. Naturforsch., B*, 1982, **37**, 412 (*cmr, B-11 nmr*)

$C_8H_{14}ClN_2OPtS^{\oplus}$ IC-006029

Chloro(1,2-diaminobenzene)(dimethyl sulfoxide) platinum(*II*)(1+)

(*1,2-Benzenediamine*-N,N')*chloro*[*sulfinylbis*[*methane*]-S] *platinum(1+), 12CI*



M 416.8 (ion)
Presumed square planar. Simplest example of many complexes with antitumour props. containing diamine and sulfoxide ligands.
Nitrate: [124442-33-7].
White solid (MeOH/Et_2O).

Farrell, N. *et al, Inorg. Chem.*, 1990, **29**, 397 (*synth, ir, Pt-195 nmr, props*)

$C_8H_{14}Cl_2O_4Ti$ IC-006030

Bis(butanoato)dichlorotitanium(*IV*), 11CI

[39218-85-4]

$(H_3CCH_2CH_2COO)_2TiCl_2$

M 292.9
Synth. by reaction of $TiCl_4$ and butanoic acid in refluxing CCl_4. Catalyst in the copolym. of α-olefins and non-conjugated dienes. Yellow, v. moisture-sensitive solid.
Py complex: [104854-01-5]. *Bis(butanoato*-O) *dichloro(pyridine)titanium*(IV), *11CI*
$C_{13}H_{19}Cl_2NO_4Ti$ M 372.0
V. moisture-sensitive yellow solid.

Japan. Pat., 72 34 588, (1972); *CA*, **79**, 79722z (*use*)
Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1986, **25**, 271 (*synth, ir, deriv*)

$C_8H_{14}Cl_2O_4Ti$ IC-006031

Dichlorobis(2-methylpropanoato-*O*)titanium(*IV*), 9CI

Dichlorobis(isobutyrato)titanium(IV), *8CI*

[19126-51-3]

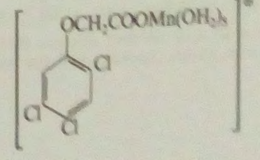
$[(H_3C)_2CHCOO]_2TiCl_2$

M 292.9
Synth. by reaction of $TiCl_4$ with excess acid. Catalyses the copolym. of α-olefins and both conjugated and unconjugated dienes (cf. Bis(butanoato) dichlorotitanium(*IV*), IC-006030).

Amaudrut, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **264**, 2156 (*synth*)
Ger. Pat., 2 112 839, (1971); *CA*, **76**, 47124c (*use*)
Japan. Pat., 74 40 633, (1974); *CA*, **83**, 44037k (*use*)

$C_8H_{14}Cl_3MnO_8^{\oplus}$ IC-006032

Pentaaqua[(2,4,5-trichlorophenoxy)acetato-*O*¹] manganese(*II*)(1+), 11CI



M 399.4 (ion)
Mn(*II*) complex of the auxin herbicide 2,4,6-trichlorophenoxyacetic acid.

2,4,5-Trichlorophenoxyacetate salt: [84076-72-2].
$C_{16}H_{18}Cl_6MnO_{11}$ M 653.9
Synth. from $MnCO_3$ and 2,4,5-trichlorophenoxyacetic acid in aq. EtOH. Colourless needles (EtOH aq.). Dec. to form Tetraaquabis(2,4,5-trichlorophenoxyacetato-O^1) manganese(*II*). IC-009281.

Kennard, C.H.L., *Inorg. Chim. Acta*, 1981, **52**, 55 (*synth*)
Smith, G. *et al*, *Inorg. Chim. Acta*, 1982, **62**, 241 (*cryst struct*)

$C_8H_{14}Cl_3N_2OTi$ IC-006033

Bis(acetonitrile)trichloro(tetrahydrofuran)titanium(*III*), 11CI
Titanium(III) *chloride bis(acetonitrile) tetrahydrofuran*
[76682-64-9]

$(H_3CCN)_2TiCl_3(THF)$

M 308.4
Distorted octahedral Ti. Synth. from $TiCl_3$.THF and MeCN.

Kohutova, M. *et al*, *Chem. Zvesti*, 1980, **34**, 740; *CA*, **94**, 113615p (*synth, ir, uv-vis, thermal anal*)
Zikmund, M. *et al*, *Chem. Zvesti*, 1982, **36**, 185; *CA*, **97**, 48348z (*magnetism*)

$C_8H_{14}Cl_6O_4Ti_2$ IC-006034

Bis[μ-(butanoato-*O*:*O'*)]hexachlorodititanium(*IV*), 11CI
[105007-72-5]

$(H_3CCH_2CH_2COO)_2Ti_2Cl_6$

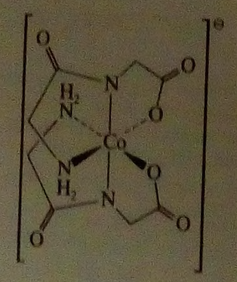
M 482.6
The dimeric formulation is based only on ir spectroscopic evidence.

Monomer: [19126-57-9]. (*Butanoato*-O)*trichlorotitanium*(IV), *11CI*
$C_4H_7Cl_3O_2Ti$ M 241.3

Kapoor, R. *et al*, *Indian J. Chem., Sect. A*, 1986, **25**, 275 (*synth, ir*)

$C_8H_{12}CoN_4O_6^{\ominus}$ IC-006035

Bis[glycylglycinato(2−)-*N*,*N*^{N},*O*']cobaltate(*III*)(1−), 9CI
[20002-42-2]



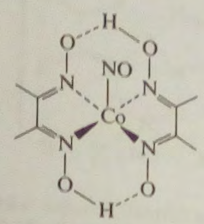
M 321.1 (ion)
mer-Octahedral; has been resolved.
Li salt: Red cryst. + $6H_2O$. Sol. H_2O.
Na salt: [15319-61-6] Red cryst. Sol. H_2O.
NH_4 salt: [15157-39-8] Red cryst. + $2H_2O$. Sol. H_2O.

Manyak, A.R. *et al*, *Arch. Biochem. Biophys.*, 1955, **59**, 373 (*synth*)
Gillard, R.D. *et al*, *Nature (London)*, 1966, **209**, 1347 (*cryst struct*)

Barnett, M.T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 367 (*cryst struct*)
Boas, C.V. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 583 (*synth, resoln, uv-vis, cd, pmr*)

$C_8H_{14}CoN_5O_5$ IC-006036

Bis(dimethylglyoximato)nitrosylcobalt
Bis[2,3-*butanedione dioximato*(1−)-N,N']*nitrosylcobalt*, *9CI*
[36509-25-8]

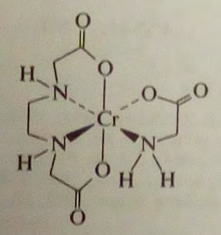


M 319.1
Square pyramidal. Model complex for vitamin B_{12} studies. Black cryst. Sol. H_2O.

Tamaki, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 171 (*synth, ir, uv*)

$C_8H_{14}CrN_3O_6$ IC-006037

(Ethylenediaminediacetato-*N*,*N'*,*O*,*O'*)(glycinato-*N*,*O*)chromium(*III*)
[[N,N'-*1,2-Ethanediylbis*[*glycinato*]](2−)-N,N',O,O'](*glycinato*-N,O)*chromium*, *11CI*
[105226-40-2]

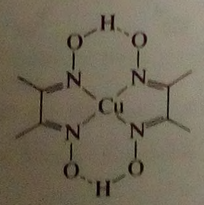


M 300.2
Cr approx. octahedral. Red cryst. + $2H_2O$. Sol. H_2O.

Green, C.A. *et al*, *Inorg. Chem.*, 1986, **25**, 4672 (*cryst struct, synth, uv-vis, nmr*)

$C_8H_{14}CuN_4O_4$ IC-006038

Bis(dimethylglyoximato)copper(*II*)
Bis[(2,3-*butanedione dioximato*)(1−)-N,N']*copper*(II), *9CI*
[14221-10-4]



M 293.7
Square planar; in solid state dimers are formed by overlap of two molecules with two Cu—O bonds. Component of reaction mixt. used for vinyl chloride polym. Cryst. (ROH).

Blink, R. *et al*, *J. Chem. Soc.*, 1958, 4536 (*ir*)

Frasson, E. *et al*, *Acta Crystallogr.*, 1959, **12**, 201 (*synth, cryst struct*)
Thabet, S.K. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 211 (*synth, ir*)
Chikira, M. *et al*, *Chem. Phys. Lett.*, 1975, **30**, 498 (*esr*)
Iwaizumi, M. *et al*, *Inorg. Chem.*, 1986, **25**, 1546 (*N-14 nmr*)

$C_8H_{14}CuO_{12}$ IC-006039

Tetraaquacopper(2+) bis(hydrogen *cis*-2-butenedioate)
Tetraaquacopper(2+) *bis(hydrogen maleate). Copper*(II) *hydrogen maleate tetrahydrate*
[22005-69-2]

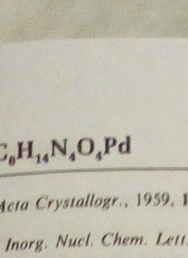
$[Cu(OH_2)_4]^{2\oplus}$ $2[HOOC—CH=CH—COO^{\ominus}]$

M 365.7
Cu coord. only by H_2O molecules to form $[Cu(OH_2)_4]_n^{2n\oplus}$ chain cations which are hydrogen bonded to the planar hydrogen maleate anions. Deep blue cryst. $\mu_{eff} = 1.96\mu_B$ (r.t.). Loses H_2O on heating >70°.

Prout, C.K. *et al*, *J. Chem. Soc. A*, 1971, 3342 (*synth, cryst struct*)
Sathyanarayana, D.N. *et al*, *Z. Anorg. Allg. Chem.*, 1971, **385**, 329 (*ir, uv*)
Mishra, H.C., *J. Inorg. Nucl. Chem.*, 1981, **43**, 605 (*synth, magnetism, ir, thermal props, cryst struct*)

$C_8H_{14}MnO_{12}$ IC-006040

Tetraaquabis[hydrogen 2-butenedioato-*O*]manganese(*II*)
Tetraaquabis(*hydrogen maleato*)*manganese*(II)
[67125-71-7]

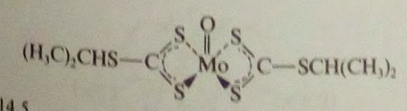


M 357.1
trans-Octahedral. Synth. from $MnCO_3$ and maleic acid. Cryst. (H_2O).

Bhat, T.R. *et al*, *Indian J. Chem.*, 1970, **8**, 275 (*synth*)
Gupta, M.P. *et al*, *Cryst. Struct. Commun.*, 1978, **7**, 179 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 140 (*rev, bibl*)

$C_8H_{14}MoOS_6$ IC-006041

Bis(isopropylthioxanthato)oxomolybdenum
Bis[*mono*(*1-methylethyl*)*carbonotrithioato*-S',S'']*oxomolybdenum*(IV), *10CI*
[65027-88-5]

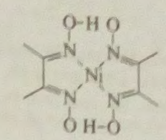


M 414.5
Pseudo-square pyramid. Obt. by dissoc. of $Mo_2O_3(S_2CSPr^i)_4$ in CS_2. Red, air-stable cryst. (CS_2/pentane 1:1). Sol. CS_2, $CHCl_3$, CH_2Cl_2, C_6H_6. Ir $\nu_{Mo=O}$ 970s cm^{-1} (CH_2Cl_2). Diamagnetic.

Hyde, J. *et al*, *Inorg. Chem.*, 1978, **17**, 414 (*cryst struct, synth, ir, uv, pmr, props*)
Miyake, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 292 (*synth, props*)

$C_8H_{14}N_4NiO_4$ IC-006042

Bis(dimethylglyoximato)nickel
Bis(2,3-*butanedione dioximato*)*nickel*, *9CI*, *8CI*. *Nickel*(II) *dimethylglyoximate*
[13478-93-8]



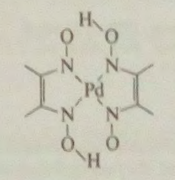
M 288.9
Square planar struct. with H-bonding between O. Solid state structure is 1-D column of stacked plates (Ni-Ni 325 pm). Used in gravimetric analysis for Ni. Ligand reactions with BF_3, $B(OR)Ph_2$ give macrocyclic complexes. Red needles ($PhNO_2$). Sol. C_6H_6, $PhNO_2$, EtOH; insol. H_2O. Subl. 250°.

[46755-15-1]

Godycki, L.E. *et al*, *Acta Crystallogr.*, 1953, **6**, 487 (*cryst struct*)
Williams, D.E. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 755 (*cryst struct*)
Orel, B. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 859 (*ir, uv, raman*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **6**, 184 (*reaction*)
Vogel's Textbook of Quantitative Inorganic Analysis, 5th Ed., Longmans, London, 1989, 462 (*synth, use*)

$C_8H_{14}N_4O_4Pd$ IC-006043

Bis(dimethylglyoximato)palladium(*II*)
Bis[(2,3-*butanedione dioximato*)(1−)-N,N']*palladium*, *9CI*
Palladium dimethylglyoxime
[14740-97-7]



M 336.6
Formed from reaction of dimethylglyoxime with Pd(*II*) salts. Formn. of this complex is the basis of a gravimetric detn. of Pd. Yellow cryst. Insol. H_2O.

Vaisbein, Zh.Yu. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 1846 (*ms*)
Hussain, M.S. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 628 (*cryst struct*)
Orel, B. *et al*, *Spectrochim. Acta, Part A*, 1980, **36**, 859 (*ir, raman, uv*)
Rios, A. *et al*, *Analyst (London)*, 1982, **107**, 737 (*synth, use*)

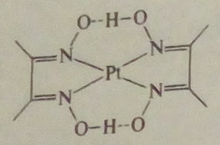
IC-006044

$C_8H_{14}N_4O_4Pt$

Bis(dimethylglyoximato)platinum(*II*)

Bis(2,3-butanedionedioximato-N,N′)platinum, 8CI

[17632-92-7]



M 425.3

Square planar struct. Has metallic conductance under 3.94 x 10^4 atm. pressure. Dark grey cryst. Sol. $PhNO_2$.

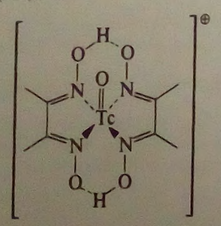
Yoshida, T., *Bull. Chem. Soc. Jpn.*, 1978, **51**, 3257 (*pe*)
Hussain, M.S., *Acta Crystallogr., Sect. B*, 1979, **35**, 628 (*synth, cryst struct*)
Shirotani, I. *et al*, *J. Solid State Chem.*, 1981, **40**, 180 (*elec cond*)
Westmore, J.B. *et al*, *Inorg. Chem.*, 1983, **22**, 902 (*synth, ms*)

IC-006045

$C_8H_{14}N_4O_5Tc^{\oplus}$

Bis(dimethylglyoximato)oxotechnetium(*V*)(1+)

Bis[2,3-butanedione dioximato(1−)-N,N′] oxotechnetium(1+), 9CI



M 345.1 (ion)

Analytical use assumes struct. shown, but Sn(*II*) reduction of $TcO_4^{\ominus}$ in presence of $dmgH_2$ gives a tris-ligand complex which also contains Tc=O—Sn bridging.

[62111-81-3]

Jasim, F. *et al*, *Talanta*, 1959, **2**, 93 (*anal*)
Deutsch, E. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1976, **73**, 4287 (*synth, cryst struct*)

IC-006046

$C_8H_{14}O_2PbS_4$

Bis(*O*-isopropyldithiocarbonato)lead(*II*)

Dithiocarbonic acid, O-(1-methylethyl)ester, lead(2+) salt, 9CI. Lead(II) *isopropylxanthate*

[5439-59-8]

$Pb[SC(S)OCH(CH_3)_2]_2$

M 477.6

Py solvate: [25721-15-7].
$C_{13}H_{19}NO_2PbS_4$ M 556.7
Cryst. (Py). Slowly loses Py in air.

Hagihara, H. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 1775 (*synth, cryst struct, Py solvate*)
Hunt, M.R. *et al*, *Aust. J. Chem.*, 1971, **24**, 53 (*ir*)

IC-006047

$C_8H_{14}O_4Pb$

Lead(*II*) butanoate

Lead butyrate. Bis(butanoato)lead

[819-73-8]

$Pb(OOCCH_2CH_2CH_3)_2$

M 381.3

Colourless scales. Insol. H_2O; sol. dil. HNO_3. Mp 90°.

▷ Poisonous.

Kharitonova, R.I. *et al*, *Zh. Neorg. Khim.*, 1975, **20**, 1823.
Indrichan, K.M. *et al*, *Zh. Neorg. Khim.*, 1984, **29**, 1450 (*ms*)

IC-006048

$C_8H_{14}O_4Rh_2^{2\oplus}$

Bis[μ-(butanoato-*O*:*O*′)]dirhodium(2+), 11CI

[89746-60-1]

$[Rh_2(O_2CCH_2CH_2CH_3)_2]^{2\oplus}$

M 380.0 (ion)

Prepd. by treating an MeCN soln. of $Rh_2(O_2CCH_2CH_2CH_3)_4$ with stoichiometric amounts of CF_3SO_3H. Not isol.

Telser, J. *et al*, *Inorg. Chem.*, 1984, **23**, 1798 (*synth, pmr, emr, props*)

IC-006049

$C_8H_{15}B_{10}BrHg$

Bromo(2-phenyl-1,2-dicarbadodecaboran(12)-1-yl) mercury, 10CI, 9CI, 8CI

(Phenyl-o-carboranyl)mercury bromide. Bromomercuri(phenyl)-o-carborane. Phenylbarenylmercury bromide

[16998-43-9]

As Chloro(2-methyl-1,2-dicarbadodecaboran(12)-1-yl) mercury, IC-003727 with

R^1 = —HgBr, R^2 = Ph

M 499.8

Solid.

Nesmeyanov, A.N. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1969, 1785 (*nqr*)
Pakhomov, V.I. *et al*, *J. Organomet. Chem.*, 1971, **29**, 15 (*cryst struct*)
Denisovich, L.I. *et al*, *J. Organomet. Chem.*, 1973, **57**, 87 (*electrochem*)
Pakhomov, V.I. *et al*, *Koord. Khim.*, 1982, **8**, 627 (*cryst struct*)

IC-006050

$C_8H_{15}N_2NbO_3$

Bis(cyano-*C*)triethoxyniobium(*V*), 11CI

[97069-03-9]

$Nb(OEt)_3(CN)_2$

M 280.1

Synth. by adding a soln. of $(EtO)_3NbCl_2$ in THF to KCN. Insol. org. solvs., H_2O.

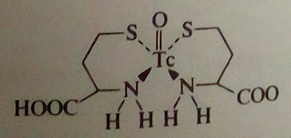
Geetha, C.N. *et al*, *Indian J. Chem., Sect. A*, 1985, **24**, 236 (*synth, ir*)

IC-006051

$C_8H_{15}N_2O_5S_2Tc$

Bis(homocysteine)oxotechnetium(*V*)

Bis(2-amino-4-mercaptobutyrato)oxotechnetium(V)



M 382.2

Tentative formulation for ill-characterised complex, which may not even be mononuclear. Synth. from $TcO_4^{\ominus}$ and an excess of ligand. Potential imaging agent.

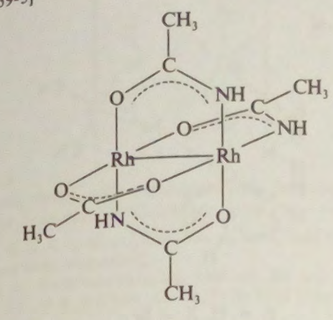
Takeda, A. *et al*, *Appl. Radiat. Isot.*, 1989, **40**, 565.

IC-006052

$C_8H_{15}N_3O_5Rh_2$

Tris[μ-(acetamidato-*N*:*O*)][μ-(acetato-*O*:*O*′)] dirhodium(*II*), 11CI

[87985-39-5]



M 439.0

Prepd. *in situ* by treating $Rh_2(OAc)_4$ with excess molten acetamide. Sol. MeCN, DMSO.

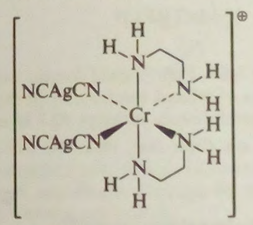
Zhu, T.P. *et al*, *Inorg. Chem.*, 1984, **23**, 2 (*synth, electrochem*)
Chavan, M. *et al*, *Inorg. Chem.*, 1984, **23**, 4538 (*electrochem, uv, esr*)

IC-006053

$C_8H_{16}Ag_2CrN_8^{\oplus}$

Bis[dicyanosilver(*I*)-*N*]bis(ethylenediamine)chromium(*III*)

Bis[μ-(cyano-C:N)]bis[(cyano-C)silver]bis(1,2-ethanediamine-N,N′)chromium(III)(1+), *11CI*



M 492.0 (ion)

For isocyano derivative, see under Bis(cyano-*N*)bis(1,2-ethanediamine-*N*,*N*′)silverchromium(2+), IC-005250.

Δ-cis-form

Perchlorate: [98585-12-7].
Synth. from aq. Δ-*cis*-$[Cr(CN)_2(en)_2]$ (ClO_4) and $AgClO_4$. Orange cryst. + $2H_2O$.

Sakaguchi, U. *et al*, *Inorg. Chim. Acta*, 1985, **101**, 23 (*cryst struct, synth*)

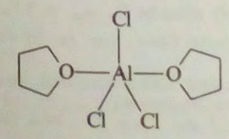
IC-006054

$C_8H_{16}AlCl_3O_2$

Trichlorobis(tetrahydrofuran)aluminium

Aluminium chloride tetrahydrofuran (1:2)

[15615-14-2]



M 277.5

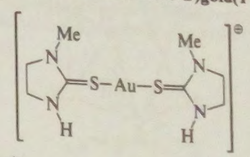
From $(Me_2N)_3SiCl$ and $AlCl_3$ in THF. Colourless moisture sensitive cryst. (Et_2O). Sol. THF, CH_2Cl_2. *cf.* Struct. of Dichlorotetrakis(tetrahydrofuran)aluminium(1+), IC-009450.

Derouault, J. *et al*, *Inorg. Chem.*, 1977, **16**, 3214 (*raman, Al-27 nmr*)
Cowley, A.H. *et al*, *Inorg. Chem.*, 1981, **20**, 1179 (*synth, cryst struct*)

IC-006055

$C_8H_{16}AuN_4S_2^{\oplus}$

Bis(1-methyl-2-imidazolidinethione-*S*)gold(1+), 11CI



M 429.3 (ion)

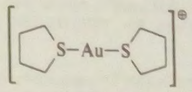
Chloride: [100011-79-8].
$C_8H_{16}AuClN_4S_2$ M 464.7
Light brown cryst. (MeOH). Mp 246-247°.

Isab, A.A. *et al*, *Polyhedron*, 1985, **4**, 1683 (*synth*)

IC-006056

$C_8H_{16}AuS_2^{\oplus}$

Bis(tetrahydrothiophene)gold(*I*)(1+)



M 373.3 (ion)

Possesses antiarthritic activity. V. useful reagent for synth. of co-ordination and organometallic complexes of Au(*I*).

Perchlorate: [69462-29-9].
Colourless cryst. (CH_2Cl_2/Et_2O). Sol. CH_2Cl_2, $CHCl_3$, Me_2CO; insol. Et_2O, hexane. Mp 113° dec. Slowly dec. at r.t.

▷ Potentially explosive.

Diiodoaurate salt: see *Iodo(tetrahydrothiophene)gold*(I), *IC-004054*

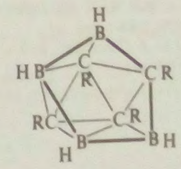
U.S. Pat., 4 112 113, (1977); *CA*, 1979, **90**, 127542s (*synth, antiarthritic activity*)
Usón, R. *et al*, *Inorg. Chim. Acta*, 1986, **112**, 205 (*synth, mössbauer*)

IC-006057

$C_8H_{16}B_4$

3,5,6,8-Tetramethyl-3,5,6,8-tetracarbaoctaborane(8), 10CI

[65230-40-2]



R = Me

M 155.4

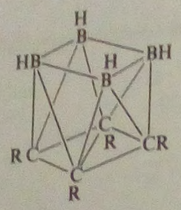
nido-. Exhibits fluxional behaviour with second-*nido*-struct., 5,6,7,8-Tetramethyl-5,6,7,8-tetracarbaoctaborane(8), IC-006058. Synth. by irradiation of $B_4H_8Fe(CO)_3$ with $H_3CC{\equiv}CCH_3$ in pentane for 18h. Clear colourless viscous liq.

Fehlner, T.P. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 8355; 1980, **102**, 3424 (*synth, ms, pmr, B-11 nmr*)
Siebert, W. *et al*, *Chem. Ber.*, 1979, **112**, 1480 (*synth, ms*)

$C_8H_{16}B_4$ IC-006058

5,6,7,8-Tetramethyl-5,6,7,8-tetracarbaoctaborane(8), 10CI

[74417-78-0]



R = Me

M 155.4

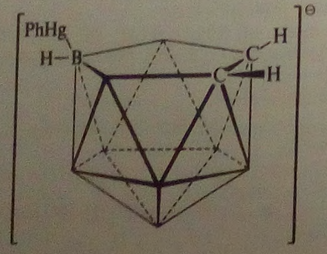
nido-. Exhibits fluxional behaviour with a second-*nido*-struct., 3,5,6,8-Tetramethyl-3,5,6,8-tetracarbaoctaborane(8), IC-006057. Synth. by irradiation of $B_4H_8Fe(CO)_3$ with $H_3CC{\equiv}CCH_3$ in pentane for 18h. Clear colourless viscous liq.

Fehlner, T.P., *J. Am. Chem. Soc.*, 1977, **99**, 8355; 1980, **102**, 3424 (*synth, ms, pmr, B-11 nmr*)
Siebert, W. *et al*, *Chem. Ber.*, 1979, **112**, 1480 (*synth*)

$C_8H_{16}B_9Hg^{\ominus}$ IC-006059

Phenyl](10-η)-undecahydro-7,8-dicarbaundecaborato(2−)]mercurate(1−), 10CI

Phenyl-(3)-1,2-dicarbollylmercury anion



M 410.1 (ion)

Me_4N salt: [71343-99-2].
Cryst. (THF/pentane or THF/hexane). Sol. H_2O, Et_2O, THF. Mp 210° dec.

[32492-37-8]

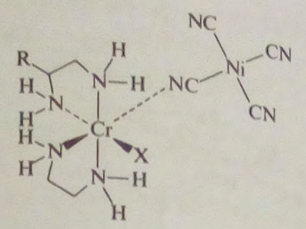
Mikhailov, B.M. *et al*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1970, 2484 (*synth, ir*)
Colquhoun, H.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 619 (*synth, pmr, B-11 nmr, ir*)

$C_8H_{16}BrCrN_8Ni$ IC-006060

Bromo[μ-(cyano-*C:N*)]bis(1,2-ethanediamine-*N,N'*)[tris(cyano-*C*)nickel(*II*)]chromium(*III*), 10CI

[*Bromobis(ethylenediamine)chromium*(III)]-μ-*cyano*(*tricyano*)*nickel*(II)

[72067-37-9]



R = H, X = Br

M 414.8

Synth. from *cis*-$[CrBr(en)_2(H_2O)]^{2\oplus}$, $2Br^{\ominus}$ + NH_4 salt of Tetrakis(cyano-*C*)nickelate(2−), IC-004541. Solid + $1H_2O$.

Ribas, J. *et al*, *Inorg. Chim. Acta*, 1979, **36**, 41.
Ribas, J. *et al*, *Transition Met. Chem.*, 1984, **9**, 287 (*synth, ir, uv*)

$C_8H_{16}BrFeO_2^{\oplus}$ IC-006061

Bromobis(tetrahydrofuran)iron(*II*)(1+)

[80679-61-4]

$[FeBr(THF)_2]^{\oplus}$

M 279.9 (ion)

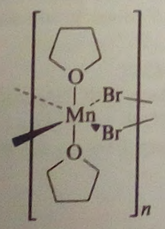
Formed in gas phase from $FeBr^{\oplus}$, itself formed from $Fe^{\oplus}$ and MeBr. A series of related species may be formed in gas phase. Two ligand dissoc. enthalpy 42.7 kJ mol^{-1}.

Kappes, M.M. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 1819.

$C_8H_{16}Br_2MnO_2$ IC-006062

Dibromobis(tetrahydrofuran)manganese(*II*)

Manganese(II) *bromide bis(tetrahydrofuran)*



M 358.9

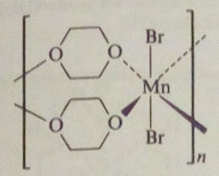
Polymeric chain struct. with octahedral Mn. Synth. from anhydrous $MnBr_2$ and THF. White or pink cryst. (THF). Reacts with $PPhMe_2$ in THF to form a complex which reversibly absorbs O_2. $\mu_{eff} = 5.8\mu_B$ (r.t.).

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 143 (*rev, bibl*)
Hosseiny, A. *et al*, *Inorg. Chim. Acta*, 1980, **39**, 227 (*synth, struct, electrochem, ir, esr, magnetism*)
Murray, B.D. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 7011 (*synth*)

$C_8H_{16}Br_2MnO_4$ IC-006063

Dibromobis(1,4-dioxane-O^1)manganese(*II*), 9CI

[20770-21-2]



M 390.9

Polymeric struct. with octahedral Mn. Prepared from $MnBr_2$ and dioxan. Colourless cryst.

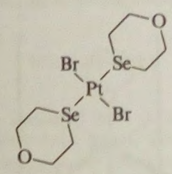
Fowles, G.W.A. *et al*, *J. Chem. Soc. A*, 1968, 1842 (*synth, ir, thermal anal, magnetism*)
Oekrug, D., *Naturwissenschaften*, 1968, **55**, 206 (*uv*)
Barnes, J.C. *et al*, *J. Chem. Soc. A*, 1970, 1442 (*synth, thermal anal*)
Barnes, J.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 923.
Barnes, J.C. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 404 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 154 (*rev, bibl*)

$C_8H_{16}Br_2O_2PtSe_2$ IC-006064

Dibromobis(1,4-oxaselenane)platinum, 10CI

Dibromobis(1-oxa-4-selenacyclohexane)platinum(II)

[60552-24-1]



M 657.0

trans-structure only found. Unusual O,Se heterocyclic ligand, coordinates through Se. Sol. CH_2Cl_2, $CHCl_3$. Cl, Pd, S analogues known.

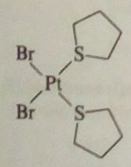
[63039-59-8]

Barnes, J.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1227; 1977, 458 (*pmr, cryst struct*)

$C_8H_{16}Br_2PtS_2$ IC-006065

Dibromobis(tetrahydrothiophene)platinum(*II*), 8CI

Dibromobis(tetramethylenesulfide)platinum



cis-form

M 531.2

Cl analogue known.

cis-form [36450-27-8]
Formed from *trans*-form at 95°. Reconverted by adding KBr to aq. Me_2CO soln. White solid. Sol. H_2O, $CHCl_3$. Mp 120°.

trans-form [36400-26-7]
Props not described.

Kukushkin, Y.N. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 1486 (*synth*)

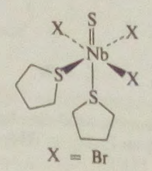
Allen, E.A. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 725 (*synth, ir, raman*)
Andronov, E.A. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 1343 (*synth, ir, dta*)

$C_8H_{16}Br_3NbS_3$ IC-006066

Tribromobis(tetrahydrothiophene)thioxoniobium(*V*), 11CI

Sulfidotribromobis(tetrahydrothiophen)niobium(V).
Thiotribromobis(tetrahydrothiophen)niobium(V)

[88475-33-6]



X = Br

M 541.0

Octahedral. Synth. from $NbBr_3S$ + tetrahydrothiophene. Orange cryst. Sol. CS_2.

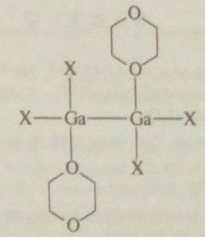
Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2251 (*synth, cryst struct*)
Baba, I.H. *et al*, *Sains Malays.*, 1984, **13**, 429 (*synth*)

$C_8H_{16}Br_4Ga_2O_4$ IC-006067

Tetrabromobis(1,4-dioxane-O^1)digallium, 11CI

Digallium tetrabromide bis(1,4-dioxan)

[68317-89-5]



X = Br

M 635.2

Ga—Ga 239.5 pm. Synth. from Ga_2Br_4 and dioxan. Colourless moisture sensitive cryst. Many similar complexes descr. See also Gallium(*I*) tetrabromogallate(*III*), IC-002019.

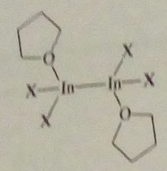
Brewer, F.M. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **23**, 45 (*similar complexes*)
Beamish, J.C. *et al*, *Inorg. Chem.*, 1979, **18**, 220 (*synth, raman*)
Small, R.W.H. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 250 (*cryst struct*)

IC-006068

$C_8H_{18}Br_4In_2O_2$

Tetrabromobis(tetrahydrofuran)diindium

[81985-67-3]



X = Br

M 693.4

Several related compds. with other ligands replacing THF descr. Synth. from In_2Br_4 + THF. White moisture-sensitive cryst. (THF).

Sinclair, I. *et al*, *Can. J. Chem.*, 1982, **60**, 690, 695 (*synth, raman*)

IC-006069

$C_8H_{16}ClCrN_8Ni$

Chloro[μ-(cyano-*C*:*N*)]bis(1,2-ethanediamine-*N*,*N'*)]tris(cyano-*C*)nickel(*II*)chromium(*III*), 10CI

Chlorobis(ethylenediamine)chromium(III)-μ-*cyano*(*tricyano*)*nickel*(II)

[72067-36-8]

As Bromo[μ-(cyano-*C*:*N*)]bis(1,2-ethanediamine-*N*,*N'*)[tris(cyano-*C*)nickel(*II*)]chromium(*III*), IC-006060 with

R = H, X = Cl

M 370.4

Synth. from *cis*-$[CrCl(en)_2(H_2O)]^{2\oplus}$, $2Br^{\ominus}$ + NH_4 salt of Tetrakis(cyano-*C*)nickelate(2−), IC-004541. Pink solid + $2H_2O$. Sol. H_2O.

Ribas, J. *et al*, *Inorg. Chim. Acta*, 1979, **36**, 41 (*synth, ir, uv*)

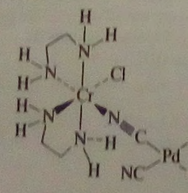
IC-006070

$C_8H_{16}ClCrN_8Pd$

Chlorobis(ethylenediamine)chromium(*III*)-μ-cyanotricyanopalladium(*II*)

Chloro(μ-*cyano*)*bis*(1,2-*ethanediamine*)[*tris*(*cyano*)*palladium*]*chromium, 11CI*

[91942-02-8]



M 418.1

Analogues known with other diamines and F, Br. Cr has *cis*-octahedral config. Synth. from Tetrakis(cyano-*C*) palladate(2−), IC-004555 + $[Cr(en)_2Cl(OH_2)]^{2\oplus}$. Pink solid. Sol. HCl (aq.). Paramagnetic.

Ribas, J. *et al*, *Transition Met. Chem.*, 1984, **9**, 287 (*synth, uv*)

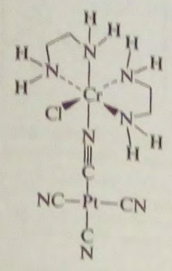
IC-006071

$C_8H_{16}ClCrN_8Pt$

Chloro(μ-cyano-*C*:*N*)bis(1,2-ethanediamine-*N*,*N'*)]tris(cyano-*C*)platinum]chromium, 11CI

[*Chlorobis*(*ethylenediamine*)*chromium*(III)]-μ-*cyano*[*tricyanoplatinum*(II)]

[91942-03-9]



M 506.7

Believed to show Pt—Pt interactions, but unconfirmed. Rose coloured solid, pink in H_2O. Sol. H_2O.

Ribas, J. *et al*, *Transition Met. Chem.*, 1984, **9**, 287 (*synth, str*)

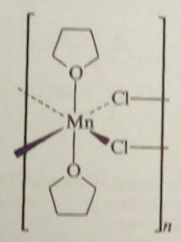
IC-006072

$C_8H_{16}Cl_2MnO_2$

Dichlorobis(tetrahydrofuran)manganese(*II*), 11CI

Manganese(II) *chloride bis*(*tetrahydrofuran*)

[70317-52-1]



M 270.0

Polymeric chain struct. with octahedral Mn(*II*). Synth. by refluxing $MnCl_2$ in THF. White cryst. (THF). Reacts with $PPhMe_2$ in THF to form a complex which reversibly absorbs O_2. μ_{eff} = 5.32μ_B (r.t.).

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 142 (*rev,bibl*)

Hosseiny, A. *et al*, *Inorg. Chim. Acta*, 1980, **39**, 227 (*synth, struct, electrochem, ir, esr, magnetism*)

IC-006073

$C_8H_{16}Cl_2O_2V$

Dichlorobis(tetrahydrofuran)vanadium(*II*), 11CI

Vanadium(II) *chloride bis*(*tetrahydrofuran*)

[21729-44-2]

$VCl_2(THF)_2$

M 266.0

Formulation uncertain. May in fact be the $[Zn_2Cl_6]^{2\ominus}$ salt of Tri-μ-chlorohexakis(tetrahydrofuran)divanadium(*II*) (1+), IC-011572. Synth. by reducing VCl_3 electrolytically in the presence of THF. Common precursor for V(*II*) compds.; cocatalyst in the carbonylation of aromatic nitro compds. by Rh salts. Green, air-sensitive solid. Paramagnetic, μ_{eff} = 3.23 (290K), 2.58μ_B (82K), θ = −107K.

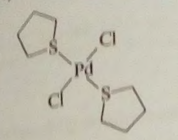
Seifert, H.J. *et al*, *J. Inorg. Nucl. Chem.*, 1968, **30**, 2081 (*synth, ir, uv-vis, magnetism*)
Unverferth, K. *et al*, *J. Prakt. Chem.*, 1979, **321**, 86 (*use*)
Girolami, G.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 1339 (*reactions*)

IC-006074

$C_8H_{12}Cl_2PdS_2$

Dichlorobis(tetrahydrothiophene)palladium(*II*)

[14221-20-6]



trans-form

M 353.6

Ir and raman indicate *trans*-struct. Synth. from Na_2PdCl_4 and tetrahydrothiophene. Yellow-orange solid (Et_2O/Me_2CO or Me_2CO at −20°). Mp 163-165°, 173°.

[26923-56-8]

Clark, R.J.H. *et al*, *J. Chem. Soc. A*, 1970, 659 (*synth, ir, raman*)
Abel, E.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1994 (*synth, pmr*)
Uson, R. *et al*, *Transition Met. Chem.*, 1980, **5**, 284.

IC-006075

$C_8H_{16}Cl_3MnO_4$

Trichlorobis(1,4-dioxan-*O*^{1})manganese(*III*), 10CI

[61301-91-5]

$MnCl_3(dioxan)_2$

M 337.5

Struct. not known. Prepared from dioxan and $MnCl_3$ in Et_2O at −50°. Red-violet flakes, light and moisture sensitive, stable below −30°. Non-electrolyte in Me_2CO. Dioxan ligands readily replaced by pyridine N-oxides and phosphine oxides.

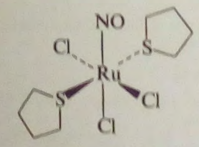
Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **349**, 45 (*synth*)
Usón, R. *et al*, *Transition Met. Chem.*, 1976, **1**, 122 (*synth, uv, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 153 (*rev, bibl*)

IC-006076

$C_8H_{16}Cl_3NORuS_2$

Trichloro(nitrosyl)bis(tetrahydrothiophene)ruthenium, 9CI

[15550-49-9]



prob. struct.

M 413.7

Octahedral. Prepd. by treating Diaquatrichloro(nitrosyl) ruthenium, IC-016865 with tetrahydrothiophene. Orange solid. Ir ν_{NO} 1850 cm^{-1}.

Fairey, M.B. *et al*, *Spectrochim. Acta*, 1964, **20**, 1757 (*ir*)
Fairy, M.B. *et al*, *J. Chem. Soc. A*, 1966, 475 (*synth*)

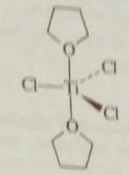
IC-006077

$C_8H_{16}Cl_3O_2Ti$

Trichlorobis(tetrahydrofuran)titanium(*III*), 11CI

Titanium(III) *chloride bis*(*tetrahydrofuran*)

[29791-08-0]



M 298.4

$TiCl_3$ dissolves in THF to form the tris-adduct, forming di-THF complex on heating to 90°. Green solid.

EtOH complex: [102511-73-9]. *Trichloro*(*ethanol*)*bis*(*tetrahydrofuran*)*titanium*(III)
$C_{10}H_{22}Cl_3O_3Ti$ M 344.5
Possesses *fac*-octahedral struct.

Zikmund, M. *et al*, *Chem. Zvesti*, 1969, **23**, 843; 1979, **33**, 180; *CA*, **74**, 27638d; **91**, 150242y (*synth, magnetism*)
Seifert, H.J. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **372**, 79 (*synth, ir*)
Plesch, G. *et al*, *Chem. Zvesti*, 1981, **35**, 613; *CA*, **96**, 45287x (*esr, ir*)
Kohutova, M. *et al*, *Proc. Conf. Coord. Chem., 10th*, 1985, 201; *CA*, **104**, 236139u (*deriv*)

IC-006078

$C_8H_{16}Cl_3O_3W$

Trichlorooxobis(tetrahydrofuran)tungsten(*V*), 11CI, 10CI, 8CI

Tungsten(V) *chloride oxide* (WCl_3O) *bis-tetrahydrofuran*

[18131-65-2]

$WOCl_3(THF)_2$

M 450.4

Octahedral. Starting material. Royal-blue solid (slow dec.). Sol. MeCN. Many analogues known with other Lewis acids, see e.g. Trichlorooxobis(triethylphosphine) tungsten(*V*), IC-008035, Trichlorooxobis(triphenylphosphine oxide-*O*) tungsten(*V*), IC-013211. μ_{eff} = 1.49μ_B (298K).

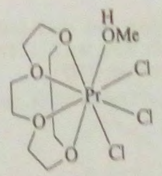
Fowles, G.W.A. *et al*, *J. Chem. Soc. A*, 1967, 671 (*synth, uv-vis, props*)
Crouch, P.C. *et al*, *J. Chem. Soc. A*, 1968, 1634 (*analogues*)
Rice, C.A. *et al*, *Inorg. Chem.*, 1981, **20**, 1996 (*reaction*)
Guy, J.T. *et al*, *Inorg. Chim. Acta*, 1985, **96**, L83 (*use*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 973 (*rev*)

IC-006079

$C_8H_{16}Cl_3O_4Pr$

Trichloro(12-crown-4)praseodymium(*III*)

(*1,4,7,10-Tetraoxacyclododecane*-O^1,O^4,O^7,O^{10}) *trichloropraseodymium*(III). *Praseodymium*(III) *chloride* (*12-crown-4*)



MeOH complex

M 423.4

Isolated by electrocrystallisation enabling H_2O molecules to be eliminated from coordination sphere.

MeOH complex:
$C_9H_{20}Cl_3O_5Pr$ M 455.5
Green cryst. Sol. MeOH. 8-Coordinate distorted sq. antiprism. Also obt. as hydrate.

Rogers, R.D. *et al, Inorg. Chim. Acta*, 1990, **172**, 173 (*synth, cryst struct*)

IC-006080

$C_8H_{16}Cl_4Ga_2O_4$

Tetrachlorobis(1,4-dioxane-O^1)digallium

Digallium tetrachloride bis(dioxan). Bis[dichloro(1,4-dioxan)gallium]

[68317-88-4]

As Tetrabromobis(1,4-dioxane-O^1)digallium, IC-006067 with

X = Cl

M 457.4
cf. Gallium(*I*) tetrachlorogallate(*III*), IC-017014. Synth. from Ga_2Cl_4 and dioxan. Colourless moisture-sensitive cryst. (dioxan). Mp 71° dec. Compd. with X = I also known.

Beamish, J.C. *et al, Inorg. Chem.*, 1979, **18**, 220 (*synth, raman, cryst struct*)

IC-006081

$C_8H_{16}Cl_4HfO_2$

Tetrachlorobis(tetrahydrofuran)hafnium(*IV*), 11Cl

Hafnium(IV) *chloride bis(tetrahydrofuran)*

[21959-05-7]

$(THF)_2HfCl_4$

M 464.5
Synth. by slow addition of dry THF to $HfCl_4$ slurry in CH_2Cl_2, or via $HfCl_4.2NMe_3$. Convenient starting material for synth. of organometallic compds. White moisture-sensitive solid. Sol. CH_2Cl_2, insol. pentane. Mp 187°.

▷ Addition of THF to solid $HfCl_4$ gives violent exothermic reaction.

[73365-24-9]

Chung, F.M. *et al, Can. J. Chem.*, 1969, **47**, 195 (*haz, thermochem*)
Wade, S.R. *et al, J. Less-Common Met.*, 1979, **68**, 105 (*synth*)
Inorg. Synth., 1982, **21**, 137 (*synth*)

IC-006082

$C_8H_{16}Cl_4In_2O_2$

Tetrachlorobis(tetrahydrofuran)diindium

[81986-28-9]

As Tetrabromobis(tetrahydrofuran)diindium, IC-006068 with

X = Cl

M 515.6
Several related compds. with other donor ligands replacing THF descr. Synth. from In_2Cl_4 + THF. White moisture-sensitive solid (THF).

Sinclair, I. *et al, Can. J. Chem.*, 1982, **60**, 695 (*synth, raman*)

IC-006083

$C_8H_{16}Cl_4MnO_8P_2$

Bis(ethyl acetate)bis(phosphorodichloridato-*O*)manganese(*II*)

[75417-30-0]

$[Mn(EtOAc)_2(O_2PCl_2)_2]_n$

M 498.9
Polymeric struct. with bridging Cl_2PO_2 groups and octahedral Mn. Synth. from MnO, $POCl_3$ and EtOAc. Moisture sensitive.

Bassett, H. *et al, J. Chem. Soc.*, 1911, **99**, 1402 (*synth*)
Danielsen, J. *et al, Acta Chem. Scand.*, 1963, **17**, 1971 (*cryst struct*)

IC-006084

$C_8H_{16}Cl_4MoO_2^{\ominus}$

Tetrachlorobis(tetrahydrofuran)molybdate(*III*)(1–)

$[MoCl_4(THF)_2]^{\ominus}$

M 381.9 (ion)
Approx. *trans*-octahedral anion. Starting material for synth. of Mo(*III*) complexes in non-aq. soln.

Ph_4P salt: [98521-67-6].
Obt. by reduction of $MoCl_4(THF)_2$ by Zn in EtOH in presence of Et_3N followed by treatment with methanolic $[PPh_4]Br$. Salmon-pink cryst. Sol. CH_2Cl_2. $\mu_{eff} = 3.90\mu_B$.

Hills, A. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1069 (*cryst struct, spectra, synth*)

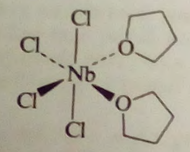
IC-006085

$C_8H_{16}Cl_4NbO_2$

Tetrachlorobis(tetrahydrofuran)niobium(*IV*), 11Cl

Niobium(IV) *chloride bis(tetrahydrofuran)*

[61247-57-2]



cis-form

M 378.9
Octahedral. Assignment of *trans*- or *cis*-geometry is based on ir or esr spectra respectively: the synthesis is the same in both cases. Synth. from $NbCl_4$ and Al in MeCN followed by recrystn. from THF. Commercially available. Pale yellow solid. Mp 93° dec. (145°).

▷ Flammable, flash point 49°.

cis-form [22943-66-4]
Pale yellow-brown solid. Paramagnetic, $\mu_{eff} = 1.55\mu_B$ (313K), $1.45\mu_B$ (93K).

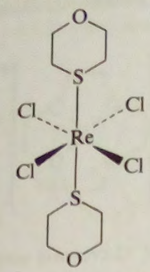
trans-form [38780-86-8]

Fowles, G.W.A. *et al, Inorg. Chem.*, 1969, **8**, 631 (*synth, ir, uv-vis, magnetism, cis-form*)
Johnson, D.P. *et al, J. Inorg. Nucl. Chem.*, 1972, **34**, 2957 (*esr, trans-form*)
Inorg. Synth., 1982, **21**, 135 (*synth*)

IC-006086

$C_8H_{16}Cl_4O_2ReS_2$

Tetrachlorobis(1,4-oxathiane)rhenium(*IV*), 8Cl



M 536.3
Presumed octahedral.

trans-form [22926-37-0]
Synth. from $ReCl_5$ and ligand. Green-yellow prisms (1,4-oxathiane).

Allen, E.A. *et al, J. Chem. Soc. A*, 1969, 788 (*synth, ir, uv, props*)

IC-006087

$C_8H_{16}Cl_4O_2Ti^{\ominus}$

Tetrachlorobis(tetrahydrofuran-*O*)titanate(*III*)(1–), 11Cl

$[(THF)_2TiCl_4]^{\ominus}$

M 333.9 (ion)
cis-Octahedral anion.

Et_4N salt: [34397-44-9].
Synth. by mixing $TiCl_3$ and Et_4NCl in THF. Green solid (THF). Paramagnetic, $\mu_{eff} = 1.78\ \mu_B$ (297K), $1.51\ \mu_B$ (77K). Reacts with $CHCl_3$ → salmon pink thermochromic substance.

Bis(tetrahydrofuran-O)lithium salt: [96443-69-5].
$C_{16}H_{32}Cl_4LiO_4Ti$ M 485.0
Synth. by reduction of $TiCl_4$ in THF with Li_3N. Active in McMurry coupling reactions. Pale blue solid (THF).

Hoff, G.R. *et al, Inorg. Chem.*, 1971, **10**, 2063 (*synth, uv-vis, esr, magnetism, Et_4N salt*)
Kilner, M. *et al, J. Chem. Soc., Chem. Commun.*, 1985, 34 (*synth, Li salt*)

IC-006088

$C_8H_{16}Cl_4O_2Ti$

Tetrachlorobis(tetrahydrofuran)titanium(*IV*), 11Cl

Titanium(IV) *chloride bis(tetrahydrofuran)*

[31011-57-1]

$(THF)_2TiCl_4$

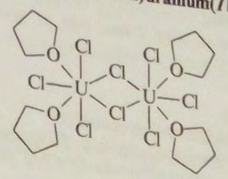
M 333.9
Octahedral. Detailed geometry not known. Synth. by adding THF to a soln. of $TiCl_4$ in CH_2Cl_2. Catalyst for the polym. of olefins. Bright yellow air-sensitive solid. Sol. CH_2Cl_2, insol. pentane. Mp 126-128°.

Perkins, P.G. *et al, J. Chem. Soc. A*, 1970, 3229 (*thermochem*)
Eur. Pat., 11 308, (1980); *CA*, **94**, 31309c (*use*)
Ikonitskii, I.V. *et al, Zh. Prikl. Spektrosk.*, 1981, **34**, 673; *CA*, **94**, 216795b (*ir*)
Inorg. Synth., 1982, **21**, 135 (*synth, ir*)

IC-006089

$C_8H_{16}Cl_4O_2U$

Tetrachlorobis(tetrahydrofuran)uranium(*IV*)



dimer

M 524.0
Dimeric with approx. pentagonal bipyramidal U.

Dimer:
$C_{16}H_{32}Cl_8O_4U_2$ M 1048.1
Air- and moisture-sensitive cryst. (THF/pentane).

Rebizant, J. *et al, Acta Crystallogr., Sect. C*, 1991, **47**, 864 (*synth, cryst struct*)

IC-006090

$C_8H_{16}Cl_4O_2V$

Tetrachlorobis(tetrahydrofuran)vanadium(*IV*), 11Cl

Vanadium(IV) *chloride bis(tetrahydrofuran)*

[12081-36-6]

$VCl_4(THF)_2$

M 336.9
Octahedral monomer. Synth. by dissolving VCl_4 in excess THF. Olefin polym. catalyst. Also active in the carbonylation of nitromesitylene. Red-brown moisture-sensitive solid. Paramagnetic, $\mu_{eff} = 1.77\mu_B$ (295K).

Bridgland, B.E. *et al, J. Inorg. Nucl. Chem.*, 1965, **27**, 383 (*synth, uv-vis, ir, magnetism*)
U.S. Pat., 4 559 318, (1985); *CA*, **104**, 187048c (*use*)
Tietz, H. *et al, Z. Chem.*, 1985, **25**, 290 (*use*)

IC-006091

$C_8H_{16}Cl_4O_2Zr$

Tetrachlorobis(tetrahydrofuran)zirconium(*IV*), 11Cl

Zirconium(IV) *chloride bis(tetrahydrofuran)*

[21959-01-3]

$(THF)_2ZrCl_4$

M 377.2
Octahedral: config. not known. Synth. by adding THF to a soln. of $ZrCl_4$ in CH_2Cl_2. White, air-sensitive solid. Mp 170-171° dec.

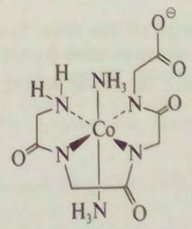
▷ A violent reaction occurs if THF is added to anhydrous $ZrCl_4$.

Westland, A.D. *et al, Can. J. Chem.*, 1970, **48**, 2871 (*synth*)
Inorg. Synth., 1982, **21**, 135 (*synth*)

IC-006092

$C_8H_{16}CoN_6O_5^{\ominus}$

Diammine[tetraglycinato(4–)]cobaltate(*III*)(1–)



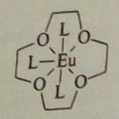
M 335.1 (ion)
Octahedral, tripeptide probably spans four planar coordination positions as shown.

NH_4 salt: $C_8H_{20}CoN_7O_8$ M 353.2
Orange solid.

Hawkins, C.J. *et al, Inorg. Chem.*, 1982, **21**, 3681 (*synth, uv, pmr, cmr*)

IC-006093

$C_8H_{16}EuN_3O_{13}$
(12-Crown-4)trinitratoeuropium(*III*)
Europium(III) *nitrate 12-crown-4. Tris(nitrato-O,O′)(1,4,7,10-tetraoxacyclododecane-O^1,O^4,O^7,O^{10})europium*
[82384-79-0]

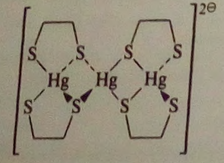


L = NO_3

M 514.1
10-Coordinate with bidentate nitrate. Colourless cryst. Sl. sol. $MeNO_2$, MeCN. Paramagnetic; μ_{eff} = 3.31μ_B. Dec. >280°; isomorphous with Nd-Lu analogues.

Bünzli, J.-C.G. *et al, Inorg. Chim. Acta*, 1982, **59**, 269; 1980, **44**, L55 (*synth, cryst struct, ir, raman*)
Inorg. Synth., 1985, **23**, 149 (*synth, ir, magnetism*)

$C_8H_{16}Hg_3S_8^{2\ominus}$ IC-006094
Tetrakis[μ-1,2-ethanedithiolato(2−)-*S:S,S′*]trimercurate(2−)



M 970.5 (ion)
Tetrahedral Hg. Synth. from $HgCl_2$ in MeOH + excess $HSCH_2CH_2SH$.
Bis-Ph_4P salt: [102502-05-6].
Cryst. (MeOH).

Henkel, G. *et al, J. Chem. Soc., Chem. Commun.*, 1985, 1498 (*synth, cryst struct*)

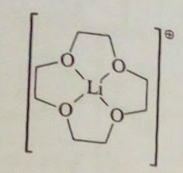
$C_8H_{16}I_4In_2O_2$ IC-006095
Tetraiodobis(tetrahydrofuran)diindium
[81985-68-4]
As Tetrabromobis(tetrahydrofuran)diindium, IC-006068 with

X = I

M 881.4
Several related complexes also descr. Synth. from In_2I_4 + THF. White moisture-sensitive cryst. (THF).

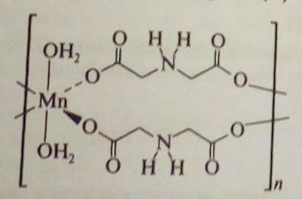
Sinclair, I. *et al, Can. J. Chem.*, 1982, **60**, 690, 695 (*synth, raman*)

$C_8H_{16}LiO_4^{\oplus}$
(12-Crown-4)lithium(1+) IC-006096
(1,4,7,10-Tetraoxacyclododecane) lithium(1+) complex, 9Cl
[57448-31-4]



M 183.1 (ion)
Synth. by reaction of 12-crown-4 with a lithium salt in MeOH.
Bis(trimethylsilyl)amide, salt: see *Lithium bis(trimethylsilyl) amide, IC-005384*
Thiocyanate salt: [57448-32-5].
Synth. from stoichiometric quantities of LiSCN and 12-crown-4 in Me_2CO. Colourless cryst. Mp 260°. $Li^{\oplus}$ lies above the plane of the crown heteroatoms. Coord. sphere completed by an anion N.
Chloride: [53894-04-5].
Bromide: [53894-03-4].
Anet, F.A.L. *et al, Acta Chem. Scand.*, 1973, **27**, 3395 (*synth, pmr, cmr, ir*)
McLachlan, R.D. *et al, Spectrochim. Acta, Part A*, 1974, **30**, 1171 (*ir, chloride, bromide*)
Pullman, A. *et al, Chem. Phys. Lett.*, 1975, **35**, 156 (*theory*)
Yanagida, S. *et al, Bull. Chem. Soc. Jpn.*, 1978, **51**, 3111 (*synth, ir, thiocyanate*)
Groth, P., *Acta Chem. Scand., Ser. A*, 1981, **35**, 463 (*struct, thiocyanate*)
Hori, K., *Tetrahedron*, 1983, **39**, 67 (*theory*)
Power, P. *et al, J. Chem. Soc., Chem. Commun.*, 1984, 358 (*struct of $LiN(SiMe_3)_2$ complex*)
Rode, B.M. *et al, Inorg. Chim. Acta*, 1985, **96**, 91 (*theory*)
Eliasson, B. *et al, J. Phys. Chem.*, 1985, **89**, 258 (*cmr, O-17, Li-7 nmr*)
Erk, C., *Spectrosc. Lett.*, 1985, **18**, 723 (*stability*)
Tsivadze, A.Yu. *et al, Zh. Neorg. Khim.*, 1986, **31**, 318 (*raman, ir, chloride, bromide, thiocyanate*)

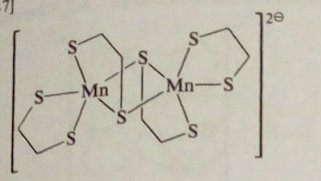
$C_8H_{16}MnN_2O_{10}$ IC-006097
Diaquabis(iminodiacetato-*O*)manganese(*II*)



M 355.1
Polymeric struct. with bridging iminodiacetate groups.

Anan'eva, N.N. *et al, Sov. J. Coord. Chem. (Engl. Transl.)*, 1975, **1**, 346 (*cryst struct*)
Anan'eva, N.N. *et al, Koord. Khim.*, 1987, **11**, 702 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 5 (*rev, bibl*)

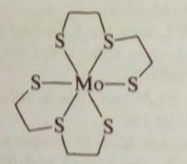
$C_8H_{16}Mn_2S_8^{2\ominus}$ IC-006098
Tetrakis(ethane-1,2-dithiolato)dimanganate(*III*)(2−)
Bis[μ-[1,2-ethanedithiolato(2−)-S:S,S′]]bis[1,2-ethanedithiolato(2−)-S,S′]manganate(III)(2−), *11Cl*
[87526-32-7]



M 478.6 (ion)
Mn atoms in distorted trigonal bipyramidal arrangement. Exists in equilibrium with $[Mn(SCH_2CH_2S)_2(solv.)_{1,2}]^{\ominus}$ in coordinating solvs. Two Mn(*III*) centres are antiferromagnetically coupled at r.t.
Bis-Et_4N salt: [87526-33-8].
Synth. by exposing $[NEt_4]_2[Mn(SCH_2CH_2S)_2]$ to the atm. in a controlled fashion. Black prisms (MeCN/THF), stable under anaerobic conditions. μ_{eff} = 3.96μ_B (298K).
Bis-Ph_4P salt: [87860-07-9].
Synth. by controlled oxidation of $[Ph_4P]_2[Mn(SCH_2CH_2S)_2]$ with air. Dark green cryst. (DMF/Et_2O).

Costa, T. *et al, Inorg. Chem.*, 1983, **22**, 4091 (*synth, cryst struct, electrochem, uv, magnetism*)
Christou, G. *et al, J. Chem. Soc., Chem. Commun.*, 1983, 558 (*synth, cryst struct, electrochem*)
Seela, J.L. *et al, Inorg. Chem.*, 1985, **24**, 4454 (*magnetism*)
Rao, C.P. *et al, Inorg. Chem.*, 1986, **25**, 428 (*synth*)
Mukherjee, R.N. *et al, Inorg. Chem.*, 1986, **25**, 2979 (*magnetism, electrochem*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 34, 42 (*rev, bibl*)

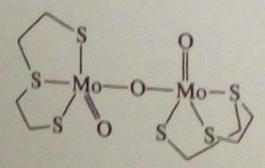
$C_8H_{16}MoS_6$ IC-006099
Bis[[2,2′-thiobis[ethanethiolato]](2−)-*S,S′,S″*]molybdenum(*IV*), 10CI
Bis[bis(2-thiolatoethyl)sulfide]molybdenum(IV)
[73952-97-3]



M 400.5
Trigonal prismatic. Synth. from $MoCl_5$ + $(HSCH_2CH_2)_2S$. Dark green cryst. (by chromatog. $Al_2O_3/CH_2Cl_2/MeOH$ 3:1). Sol. CH_2Cl_2. Undergoes reversible $1e^{\ominus}$ oxidation at +0.53V and a reversible $1e^{\ominus}$ reduction at −1.07V.

Hyde, J. *et al, J. Chem. Soc., Chem. Commun.*, 1980, 204 (*cryst struct, synth, ir, uv*)

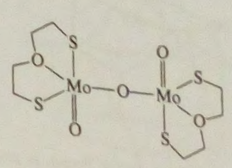
$C_8H_{16}Mo_2O_3S_6$ IC-006100
μ-Oxodioxobis[[2,2′-thiobis[ethanethiolato]](2−)-*S,S′,S″*]dimolybdenum(*V*), 11CI, 10CI



M 544.4
The geometries about Mo are severely distorted from either idealised trigonal pyramidal or square pyramidal.
Cryst.

Hyde, J.R. *et al, Cryst. Struct. Commun.*, 1982, **11**, 929 (*cryst struct*)

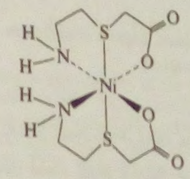
$C_8H_{16}Mo_2O_5S_4$
μ-Oxodioxobis[[2,2′-oxybis[ethanethiolato]](2−)-*O,S,S′*]molybdenum(*V*), 11CI IC-006101
[83915-05-3]



M 512.3
5-Coordinate Mo with Mo=O 173.8, Mo—O_{term} 214.7, Mo—O_{br} 190.0, Mo—S 236.5, 237.9 pm. Cryst.

Hyde, J.R. *et al, Cryst. Struct. Commun.*, 1982, **11**, 929 (*cryst struct*)

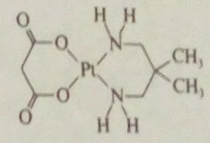
$C_8H_{16}N_2NiO_4S_2$
Bis[[(2-aminoethyl)thio]acetato-N,O,S]nickel(*II*), 8CI IC-006102
Bis(5-amino-3-thiapentanoato)nickel(II). *Bis(5-amino-2-thiovalerato)nickel*(II)
[16827-65-9]



M 327.0
Approx. octahedral. Blue cryst. (H_2O).

Rose, N.J. *et al, Inorg. Chem.*, 1967, **6**, 1431 (*synth, ir*)

$C_8H_{16}N_2O_4Pt$ IC-006103
2,2-Dimethyl-1,3-propanediamine(propanedioato)platinum, 10CI
(1,3-Diamino-2,2-dimethylpropane)(malonato)platinum(II)
[72968-07-1]

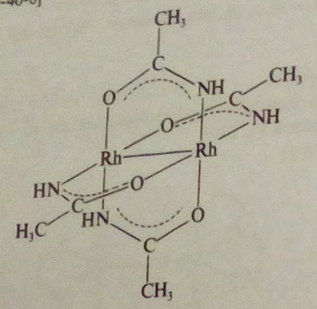


M 399.3
Square planar struct.; diamine has chair, malonate has boat configurations. Potential anticancer agent. White solid. Sol. H_2O. Diamine known as DMDAP. Other $[PtX_2(DMDAP)]$ complexes also known.
▷ TP2497700.

van Kranligen, C.G. *et al, Inorg. Chem.*, 1980, **19**, 1481.

IC-006104

$C_8H_{16}N_4O_4Rh_2$
Tetrakis[μ-(acetamidato-*N*:*O*)]dirhodium(*II*), 11CI
[87985-40-8]



M 438.0
Analogue of $M_2(RCO_2)_4$ struct. Prepd. *in situ* by treating $Rh_2(OAc)_4$ with excess molten acetamide. Sol. MeCN, DMSO.

Zhu, T.P. *et al*, *Inorg. Chem.*, 1984, **23**, 2 (*synth, electrochem*)
Chavan, M. *et al*, *Inorg. Chem.*, 1984, **23**, 4538 (*electrochem, uv, esr*)

IC-006105

$C_8H_{16}N_4O_8Pt^{2\ominus}$
Tetrakis(glycinato-*N*)platinate(*II*), 8CI
[17084-16-1]

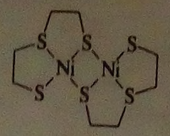
$[Pt(NH_2CH_2COO)_4]^{2\ominus}$

M 491.3 (ion)
Square planar struct. Ligand coordinates through N.
Di-K salt: [21791-04-8].
Sol. H_2O.
[66018-36-8]

Grinberg, A.A. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1935, **2**, 485 (*synth*)
Volshtein, L.M. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1960, **5**, 840 (*synth*)
Erickson, L.E. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 6371 (*pmr*)
Erickson, L.E. *et al*, *Inorg. Chem.*, 1978, **17**, 1701 (*cmr*)

IC-006106

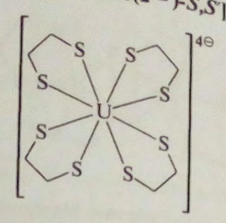
$C_8H_{16}Ni_2S_6$
Bis[bis(2-mercaptoethyl) sulfide]dinickel(*II*)
Bis[μ-[[2,2′-*thiobis*[*ethanethiolato*]](2−)-S:S,S^1,S^2]]*dinickel*, *9CI*
[21590-66-9]



M 421.9
Square planar at Ni, molecule is bent at the S bridges, which may give rise to Ni—Ni interactions. Ikram states erroneously that the molecule is planar. Synth. from $(HSCH_2CH_2)_2S$, $NiSO_4.(NH_4)_2SO_4$ or $NiSO_4$ and NH_3. Dark red cryst. ($CHCl_3$/EtOH or $CHCl_3$). V. sol. halogenated solvs. $\mu_{eff} = 0.36\mu_B$.
[36488-62-7, 39358-80-0]

Harley-Mason, J., *J. Chem. Soc.*, 1952, 146 (*synth*)
Barclay, G.A. *et al*, *Aust. J. Chem.*, 1968, **21**, 2669 (*synth, props, uv*)
Barclay, G.A. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 1262 (*cryst struct*)
Ikram, M. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 59 (*ir*)

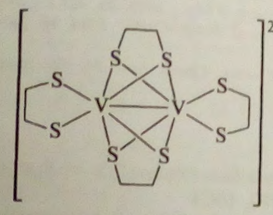
$C_8H_{16}S_8U^{4\ominus}$
IC-006107
Tetrakis[ethane-1,2-dithiolato(2−)-*S*,*S*′]uranate(*IV*)(4−)



M 606.7 (ion)
8-Coord. dodecahedral anion; fluxional. Rare example of U solely bonded to *S*.
Tetrakis[(*1,2-dimethoxyethane*)*lithium*(*1+*)] *salt:* [130221-30-6].
Air-sensitive apple-green prisms + dimethoxyethane. Sol. THF, dimethoxyethane.

Tatsumi, K. *et al*, *Inorg. Chem.*, 1990, **29**, 4928 (*synth, pmr, cryst struct, uv-vis*)

$C_8H_{16}S_8V_2^{2\ominus}$
IC-006108
Bis[μ-[1,2-ethanedithiolato(2−)-*S*,*S*′:*S*,*S*′]]bis[1,2-ethanedithiolato(2−)-*S*,*S*′]divanadate(*III*)(2−), 11CI
Tetrakis(*1,2-ethanedithiolato*)*divanadate*(III)
[87145-61-7]

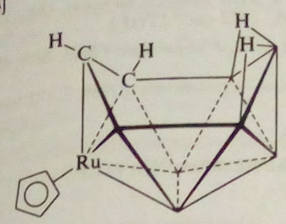


M 470.6 (ion)
V—V 260 pm.
Bis-Et_4N salt: [87145-62-8].
Synth. from VCl_3 and Na_2L in MeOH and adding $[Et_4N]Cl$. Red-brown solid (MeCN).
Bis-Ph_4P salt: [87495-20-3].
Synth. like the Et_4N salt. Black solid (DMF/MeCN/Et_2O).
Bis-Ph_4P salt, tetrakis-MeOH complex: [87495-21-4].
Synth. from VCl_3, the ligand and $[Ph_4P]Br$ in MeOH. Red-brown solid.

Szeymies, D. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 885 (*synth, cryst struct, Ph_4P/MeOH salt*)
Dorfman, J.R. *et al*, *Inorg. Chem.*, 1983, **22**, 3179 (*synth, cryst struct, Et_4N salt*)
Wiggins, R.W. *et al*, *J. Chem. Soc., Chem. Commun.*, 1983, 1313 (*synth, cryst struct, Ph_4P salt*)
Mukherjee, R.N. *et al*, *Inorg. Chem.*, 1986, **25**, 2979 (*electrochem*)

IC-006109

$C_8H_{17}B_7Ru$
(η⁶-Benzene)[η⁵-undecahydrodicarbanonaborato(2−)]ruthenium, 11CI
[94904-50-4]

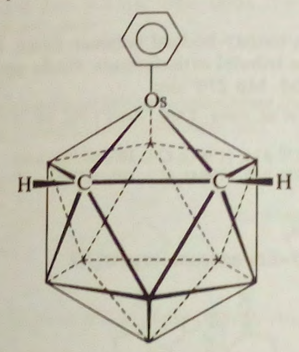


M 289.9
nido-. Yellow cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2, $CHCl_3$. Mp 149-152° dec.

Hanusa, T.P. *et al*, *Inorg. Chem.*, 1985, **24**, 787 (*synth, pmr, B-11 nmr, struct*)

IC-006110

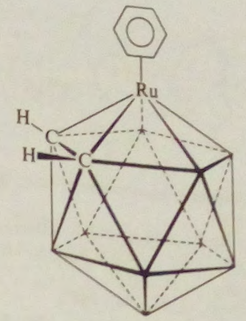
$C_8H_{17}B_9Os$
(η⁶-Benzene)[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]osmium, 11CI
3-η⁶-Benzene-1,2-dicarba-3-osmadodecaborane(11)
[94904-52-6]



M 400.7
closo-. Air-stable colourless cryst. (Me_2CO/hexane). Sol. MeCN. Mp 280-283° dec.

Hanusa, T.P. *et al*, *Inorg. Chem.*, 1985, **24**, 787 (*synth, pmr, B-11 nmr, ms*)

$C_8H_{17}B_9Ru$
IC-006111
(η⁶-Benzene)[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]ruthenium, 11CI
3,1,2-(η⁶-Benzene)$RuC_2B_9H_{11}$
[82704-20-9]



M 311.5
closo-. Yellow cryst. (Me_2CO/hexane). Sol. CH_2Cl_2. Mp 308° dec.

Hanusa, T.P. *et al*, *Polyhedron*, 1982, **1**, 77 (*synth, pmr, ir, ms*)
Garcia, M.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 2343 (*synth, cryst struct, pmr, B-11 nmr, ir*)

IC-006112

$C_8H_{17}Cl_2O_3Ti$
Dichlorohydroxybis(tetrahydrofuran)titanium(*III*), 11CI
[87918-52-3]

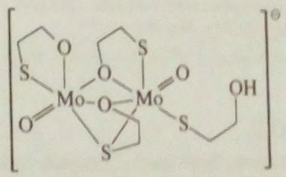
$TiCl_2(OH)(THF)_2$

M 280.0
This compd. results from studies of the interaction of Chrysotile asbestos with $TiCl_3$, thus $TiCl_3$ and Chrysotile are mixed with THF and refluxed, some of the titanium is adsorbed on the fibres. $TiCl_2(OH)(THF)_2$ cryst. from the THF. Blue, air-sensitive solid.

Cozak, D. *et al*, *Can. J. Chem.*, 1983, **61**, 2753 (*synth, pmr*)

IC-006113

$C_8H_{17}Mo_2O_6S_4^{\ominus}$
Tris[2-mercaptoethanolato(2−)][(2-mercaptoethanolato)dioxodimolybdate(*V*)](1−)
[μ-[2-*Mercaptoethanolato*(2−)-O:O,S]][μ-[2-*mercaptoethanolato*(2−)-O:O,S:S]](2-*mercaptoethanolato*-S)[2-*mercaptoethanolato*(2−)-O,S]*dioxodimolybdate*(1−), *10CI*



M 529.3 (ion)
Tripropylammonium salt: [69532-67-8].
Yellow cryst. (1-propanol/EtOH 2:5 at 0°). Sol. common alcohols, aprotic solvs. Ir $\nu_{Mo=O}$ 944, 939, 918sh cm^{-1} (nujol).

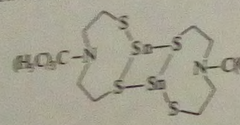
Boyd, I.W. *et al*, *Inorg. Chem.*, 1979, **18**, 1875 (*synth, cryst struct, ir*)

$C_9H_{17}NS_2Sn$ IC-006114

5-*tert*-Butyl-5-aza-2,8-dithia-1-stannabicyclo[3.3.0^{1,5}]octane

6-(1,1-Dimethylethyl)tetrahydro-4H-1,3,6,2-dithiazastannocin-2-ylidene

[88154-40-9]



dimer

M 310.0

Dimeric in solid state, monomeric in soln. In monomer, N is coord. to Sn.

Dimer: [95461-74-8]. *Bis[μ-[[2,2′-[[1,1-dimethylethyl)imino]bis(methanethiolato)](2−)-N,S,S′:S]]distin, 11Cl*

$C_{18}H_{36}N_2S_4Sn_2$ M 620.1

Colourless cryst. (C_6H_6). Mp 248°.

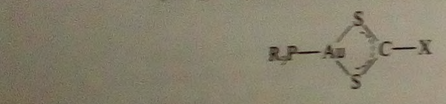
Taschach, A. *et al. Z. Anorg. Allg. Chem.*, 1983, **502**, 158 (*synth, Sn-119 nmr, cnr, pmr, mössbauer*)

Ivakochat, K. *et al. J. Organomet. Chem.*, 1985, **281**, 173 (*cryst struct*)

$C_9H_{18}AuOPS_2$ IC-006115

***O*-Methyldithiocarbonato(triethylphosphine)gold(*I*)**

(O-Methylcarbonodithioato-S,S′)(triethylphosphine)gold(I). (Methylxanthato)(triethylphosphine)gold(I)



R = Et, X = OMe

M 422.3

Cryst., dec. on standing and on recryst. Mp 66-67°.

Kowala, C. *et al. Aust. J. Chem.*, 1966, **19**, 999 (*synth*)

$C_9H_{18}AuS_2^{\ominus}$ IC-006116

Bis(*tert*-butylthiolato)aurate(*I*)

Bis(2-methylpropanethiolato)aurate(1−), 10Cl

$[(H_3C)_3CSAuSC(CH_3)_3]^{\ominus}$

M 375.3 (ion)

Ph_4P salt: [77418-55-4].

Yellow cryst. (Me_2CO). Mp 163-170°.

Bis(triphenylphosphine)iminium salt: [77424-95-4].

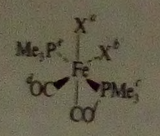
Cryst. (aq. EtOH). Mp 168-170°.

Bowmaker, G.A. *et al. J. Chem. Soc., Dalton Trans.*, 1981, 267 (*synth*)

$C_9H_{18}Br_2FeO_2P_2$ IC-006117

Dibromodicarbonylbis(trimethylphosphine)iron, 9Cl, 8Cl

[22624-30-2]



ab-dibromo-*df*-dicarbonyl-*ce*-diphosphine-*form*

X = Br

M 423.8

ab*-dibromo-*df*-dicarbonyl-*ce*-diphosphine-*form [62075-70-1]

Yellow cryst. Dec. before melting.

ab*-dicarbonyl-*ce*-dichloro-*df*-diphosphine-*form [62075-76-7]

di-trans,cis-*form*

Yellow cryst. Dec. before melting.

Pankowski, M. *et al. Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1968, 267 (*ir*)

Pankowski, M. *et al. J. Organomet. Chem.*, 1977, **125**, 231 (*synth, ir, nmr*)

$C_9H_{18}Cl_2N_2O_2Zn$ IC-006122

Dichlorobis(*N,N*-dimethylacetamide-*O*)zinc(*II*)

Zinc(II) chloride bis(N,N-dimethylacetamide-O)

[12555-56-5]

$[Me_2NC(CH_3)=O]_2ZnCl_2$

M 310.5

Tetrahedral at zinc. White cryst. Sol. $CHCl_3$. Mp 119-120°. Loses ligand on heating.

[15621-53-1]

Bull, W.E. *et al. Inorg. Chem.*, 1963, **2**, 303 (*synth*)

Canty, A.J. *Can. J. Chem.*, 1966, **44**, 1881 (*pmr, ir*)

Hennig, M. *et al. Acta Crystallogr., Sect. B*, 1974, **30**, 1289 (*cryst struct*)

Trofimov, A.Yu. *et al. Koord. Khim.*, 1977, **3**, 183 (*ir, raman*)

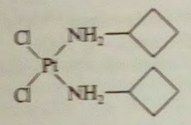
de Simoni, I. *et al. J. Chem. Soc., Dalton Trans.*, 1980, 156 (*heat of formn*)

Berdiev, A. *et al. Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1985, **30**, 1316 (*ir, thermal anal*)

$C_9H_{18}Cl_2N_2Pt$ IC-006123

Bis(aminocyclobutane)(dichloro)platinum(*II*)

Dichlorobis(cyclobutanamine)platinum, 9Cl



cis-form

M 408.2

cis-form easily converted to *trans*- by recrystallisation in Me_2CO.

***cis*-form** [38780-37-9]

Pale yellow cryst. Sol. polar org. solvs.

▷TP2195000.

***trans*-form** [76173-93-8]

Sol. polar org. solvs.

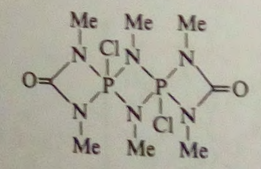
Connors, T.A. *et al. Chem. Biol. Interact.*, 1972, **5**, 415 (*synth*)

Lock, C.J.L. *et al. Inorg. Chem.*, 1981, **20**, 1817 (*cryst struct*)

$C_9H_{18}Cl_2N_4O_2P_2$ IC-006124

4,6-Dichloro-1,3,5,7,9,10-hexamethyl-1,3,5,7,9,10-hexaaza-4,6-diphospha(4,6-P^V)dispiro[3.1.3.1]decane-2,8-dione, 8Cl

[25674-41-3]



M 363.1

Cryst. ($CHCl_3$). Mp 178-180° dec.

Becke-Goehring, M. *et al. Z. Anorg. Allg. Chem.*, 1970, **372**, 285 (*synth, ir, ms, pmr, P-31 nmr*)

$C_9H_{18}ClO_2Ti$ IC-006118

Dibutoxychlorotitanium(*III*), 11Cl

[32448-94-5]

$TiCl(OCH_2CH_2CH_2CH_3)_2$

M 229.5

Synth. from $TiCl_3$ and excess tributyl orthoformate. Brown solid. Mp 280° dec.

Giannetti, E. *et al. Inorg. Chim. Acta*, 1983, **74**, 215 (*synth, ir*)

$C_9H_{18}ClO_2V$ IC-006119

Dibutoxychlorovanadium(*III*), 11Cl

[88092-82-4]

$VCl(OCH_2CH_2CH_2CH_3)_2$

M 232.6

Ir suggests a butoxy-bridged polymer. Synth. from VCl_3 and excess tributyl orthoformate. Olefin polym. catalyst. Green solid. Mp 270° dec.

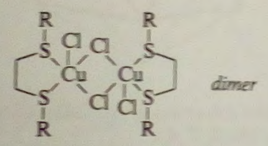
Giannetti, E. *et al. Inorg. Chim. Acta*, 1983, **74**, 215 (*synth, ir, struct*)

U.S. Pat., 4 579 834, (1984); *CA*, **105**, 6998q (*use*)

U.S. Pat., 4 579 835, (1984); *CA*, **105**, 6999r (*use*)

$C_9H_{18}Cl_2CuS_2$ IC-006120

Dichloro(4,7-dithiadecane)copper(*II*)



dimer

$R = CH_2CH_2CH_3$

M 312.8

Dimeric in solid state.

Dimer: [99727-68-1]. *Di-μ-chlorodichlorobis[1,1′-[1,2-ethanediylbis(thio)]bis[propane]-S,S′]dicopper, 11Cl*

$C_{16}H_{36}Cl_4Cu_2S_4$ M 625.6

Dark green needles (MeOH). Cu-Cl_{bridge} 266.3 pm.

Hatfield, W.E. *et al, Inorg. Chem.*, 1986, **25**, 558 (*cryst struct, magnetism, synth, uv-vis, esr*)

$C_9H_{18}Cl_2FeO_2P$ IC-006121

Dicarbonyldichlorobis(trimethylphosphine)iron

[23540-34-3]

As Dibromodicarbonylbis(trimethylphosphine)iron, IC-006117 with

X = Cl

M 303.9

ab*-dicarbonyl-*df*-dichloro-*ce*-diphosphine-*form [62075-77-8]

di-cis,cis,trans-*form*

Red-brown solid. Dec. before melting.

af*-dibromo-*bc*-dicarbonyl-*cd*-diphosphine-*form [62075-75-6]

trans,cis,cis-*form*

Red-brown cryst. (CH_2Cl_2/hexane). Dec. before melting. Ir ν_{CO} 2025, 1972 cm^{-1} (THF).

Pankowski, M. *et al. J. Organomet. Chem.*, 1977, **125**, 231 (*synth, ir, nmr*)

Cardaci, G. *et al, Organometallics*, 1988, **7**, 172 (*synth, ir*)

$C_9H_{18}Cl_2O_2Ti$ IC-006125

Dibutoxydichlorotitanium(*IV*), 11Cl

[1790-25-6]

$Ti_2Cl_4(OCH_2CH_2CH_2CH_3)_4$ (*dimer*)

M 265.0

Dimeric, as is the BuOH compd. but detailed geometries are not known. Synth. from $TiCl_4$ + $(BuO)SiR_3$. Catalyses the polym. of ethylene and block copolym. of ethylene and propylene. Component in a rapid response photosensitive soln.

Dimer: Tetrabutoxytetrachlorodititanium(IV)

$C_{16}H_{36}Cl_4O_4Ti_2$ M 530.0

Bis-urea complex: [32755-70-7]. *Dibutoxydichlorobis(urea)titanium(IV)*

Does not rapidly hydrol. in the cold. Sol. H_2O.

Martin, R.L. *et al. J. Chem. Soc.*, 1961, 2947 (*dimer formn*)

Brown, R.N. *et al. J. Chem. Soc.*, 1963, 734 (*deriv*)

Japan. Pat., 76 06 285, (1971); *CA*, **75**, 76191f (*deriv*)

U.S. Pat., 4 173 521, (1979); *CA*, **92**, 155914z (*photosensitive soln*)

Ger. Pat., 3 447 297, (1986); *CA*, **105**, 171282g (*synth*)

Japan. Pat., 61 47 712, (1986); *CA*, **105**, 153688n (*use*)

$C_9H_{18}Cl_2O_2Ti$ IC-006126

Di-*tert*-butoxydichlorotitanium(*IV*)

Dichlorobis(2-methyl-2-propanolato)titanium(IV), 11Cl

[17022-82-1]

$Ti_2Cl_4[OC(CH_3)_3]_4$ (*dimer*)

M 265.0

Dimeric by analogy with Dibutoxydichlorotitanium(*IV*), IC-006125. Synth. from $TiCl_4$ + *tert*-butanol and Et_3N. Catalyst for olefin polym.

Dimer:

$C_{16}H_{36}Cl_4O_4Ti_2$ M 530.0

Rafikov, S.R. *et al. Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1975, 1615; *CA*, **83**, 193805m (*use, polym catalyst*)

Florjanczyk, Z. *et al, Makromol. Chem.*, 1977, **178**, 1915 (*synth, use, copolym*)

Japan. Pat., 58 162 608, (1983); *CA*, **100**, 192523u (*use, polym catalyst*)

$C_9H_{18}Cl_2O_2Ti$ IC-006127

Dichlorobis(2-methyl-1-propanolato)titanium(*IV*), 11Cl

Diisobutoxydichlorotitanium(IV)

[14180-16-6]

$Ti_2Cl_4[OCH_2CH(CH_3)CH_3]_4$ (*dimer*)

M 265.0

Dimeric by analogy with Dibutoxydichlorotitanium(*IV*), IC-006125. Synth. from $TiCl_4$ + $(^tBuO)SiR_3$. Reported as a catalyst for olefin polym.

Dimer:

$C_{16}H_{36}Cl_4O_4Ti_2$ M 530.0

Ger. Pat., 2 125 074, (1971); *CA*, **76**, 114512t (*use, polym catalyst*)

Czaja, K. *et al, Polimery (Warsaw)*, 1981, **26**, 209; *CA*, **96**, 35769h (*use, polym, catalyst*)

Ger. Pat., 3 447 297, (1986); *CA*, **105**, 175282g (*synth*)

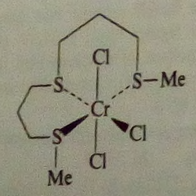
IC-006128

$C_8H_{18}Cl_3CrS_3$

[Bis(3-methylthiopropyl) sulfide]trichlorochromium(*III*)

Trichloro[1,1′-thiobis[3-(methylthio)propane]-S,S′,S″]chromium(III), *11CI. Trichloro(2,6,10-trithiaundecane)chromium*

[89655-03-8]



M 368.7

mer-Octahedral at Cr (by ir). Green moisture-sensitive solid. Br_3 and I_3 analogues known.

Gray, L.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 47 (*synth, props, ir*)

IC-006129

$C_8H_{18}Cl_3N_2Re$

Bis(*tert*-butylimido)trichlororhenium(*VII*)

Trichlorobis[2-methyl-2-propanaminato(2−)]rhenium(VII), *11CI*

[83487-31-4]

$ReCl_3[NC(CH_3)_3]_2$

M 434.8

Assumed tbp struct. with imido ligands in equatorial position. Synth. from Tris(*tert*-butylimido)(trimethylsilanolato)rhenium(*VII*), IC-009144 and HCl in CH_2Cl_2. Orange cryst. (Et_2O).

Edwards, D.S. *et al*, *Organometallics*, 1983, **2**, 1505 (*synth, nmr, struct, props*)

IC-006130

$C_8H_{18}Cl_5N_2Nb$

(Acetonitrile)pentachloro(triethylamine)niobium(*V*)

(Acetonitrile)pentachloro(N,N-*diethylethanamine*)*niobium*(V), *11CI. Niobium*(V) *chloride acetonitrile triethylamine complex*

[81900-60-9]

$NbCl_5(NEt_3)(NCCH_3)$

M 412.4

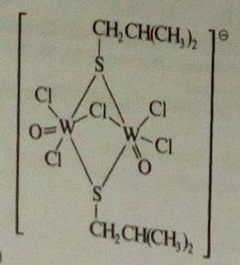
A number of amine and phosphine analogues have been described. Synth. from $NbCl_5$ and Et_3N in MeCN.

Buslaev, Yu.A., *Koord. Khim.*, 1982, **8**, 457; *CA*, **96**, 227995j (*synth*)

IC-006131

$C_8H_{18}Cl_5O_2S_2W_2^{\ominus}$

μ-Chlorotetrachlorobis[μ-(2-methyl-1-propanethiolato)]dioxoditungstate(1−), 11CI



M 755.3 (ion)

First triply-bridged oxotungsten(V) dimer. W—W 285.4 pm.

Ph_4As salt: [80288-48-8].

Red cryst. (CH_2Cl_2).

Patel, V.D. *et al*, *Inorg. Chem.*, 1982, **21**, 1383 (*synth, ir, nmr, uv, cryst struct*)

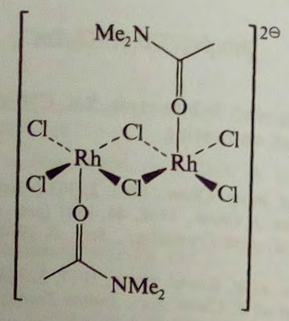
IC-006132

$C_8H_{18}Cl_6N_2O_2Rh_2^{2\ominus}$

Di-μ-chlorotetrachlorobis(*N,N*-dimethylacetamide-*O*)dirhodate(*II*)(2−), 9CI

Hexachlorobis(dimethylacetamide)dirhodate(II)(2−)

[59830-20-5]



M 592.7 (ion)

Prob. struct. based on spectroscopic data.

Bis-Ph_4P salt: Green solid. Sol. $CHCl_3$.

James, B.R. *et al*, *Coord. Chem. Rev.*, 1975, **16**, 153 (*synth, ir, uv, esr*)

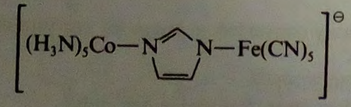
IC-006133

$C_8H_{18}CoFeN_{12}^{\ominus}$

Pentakis(cyano-*C*)[μ-(1*H*-imidazolato-N^1:N^3)](pentaamminecobaltate)ferrate(1−), 10CI

Pentaamminecobalt(III)-μ-*imidazolato*(*pentacyano*)*ferrate*(II)

[77137-30-5]



M 397.0 (ion)

Prepd. in soln., not isol.

Szecsy, A.P. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 1679 (*synth, kinetics*)

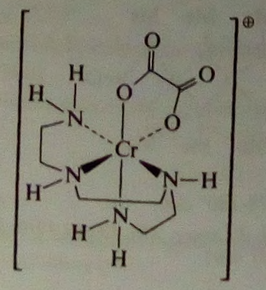
IC-006134

$C_8H_{18}CrN_4O_4^{\oplus}$

Oxalato(triethylenetetramine)chromium(*III*)(1+), 8CI

(1,8-Diamino-3,6-diazaoctane)oxalatochromium(III)(1+), [N,N′-*Bis*(2-*aminoethyl*)-1,2-*ethanediamine*-N,N′,N″,N‴][*ethanedioato*(2−)-O,O′]*chromium*(1+), *11CI, 10CI*

[81968-09-4]



cis,β-*form*

M 286.2 (ion)

Previously thought to have *cis*-α config. (House 1966), now believed (House 1982) to be *cis*-β. Used in synth. of Cr(trien)Cl_2. λ_{max} 370, 495 nm.

Bromide: [16060-20-1].

Synth. from $K_3[Cr(ox)_3].3H_2O$ + trien + KBr in H_2O. Orange red cryst. Sol. H_2O.

Perchlorate: [20097-09-0].

Synth. from oxalic acid + $Na_2Cr_2O_7$ + trien + $NaClO_4$. Pink solid. Sl. sol. H_2O. Isomer with enantiomerically pure tetradentate ligand also synth.

[81968-10-7]

House, D.A. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 2156 (*synth, uv-vis, ir, props*)

Garner, C.S. *et al*, *Transition Met. Chem.*, 1970, **6**, 59 (*rev*)

House, D.A., *Aust. J. Chem.*, 1982, **35**, 659 (*cd, uv-vis*)

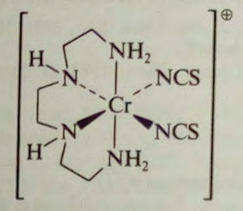
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 808 (*rev*)

IC-006135

$C_8H_{18}CrN_6S_2^{\oplus}$

Diisothiocyanato(triethylenetetramine)chromium(*III*)(1+)

[N,N′-*Bis*(2-*aminoethyl*)-1,2-*ethanediamine*-N,N′,N″,N‴]*bis*(*thiocyanato*-N)*chromium*(1+), *11CI.* (1,8-*Diamino*-3,6-*diazaoctane*)*dithiocyanatochromium*(III)



M 314.3 (ion)

Octahedral cation.

cis*-α-*form

λ_{max} 372, 488 nm. In conc. HCl with Cl_2 at 0° → violet soln. of *cis*, α-Dichloro(triethylenetetramine)chromium(*III*)(1+), IC-005315.

Thiocyanate: [88118-61-0].

Obt. by slow substitution of *cis*, β-form of Dichloro(triethylenetetramine)chromium(*III*)(1+), IC-005315 by $SCN^{\ominus}$. Orange cryst. Spar. sol. H_2O; sol. Me_2CO, MeOH.

Chloride: Obt. from Me_2CO soln. of corresp. SCN salt with HCl. Yellow orange solid. Sol. H_2O, insol. Me_2CO, MeOH.

House, D.A. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 2156 (*synth, uv-vis, ir, props*)

House, D.A. *et al*, *Inorg. Chim. Acta*, 1983, **74**, 179 (*uv-vis, cd*)

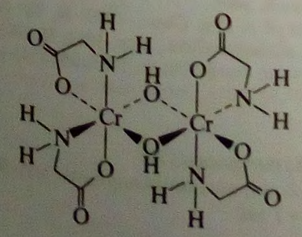
IC-006136

$C_8H_{18}Cr_2N_4O_{10}$

Tetrakis(glycinato-*N,O*)di-μ-hydroxydichromium(*III*), 11Cl, 10CI, 9CI

Di-μ-hydroxobis[*bis*(*glycinato*)*chromium*(III)]

[36926-80-4]



M 434.2

Octahedrally coordinated Cr. Pale orange cryst.

[29970-83-0]

Veal, J.T. *et al*, *Inorg. Chem.*, 1973, **12**, 342 (*cryst struct, magnetism, esr*)

Baca, A.G. *et al*, *J. Lumin.*, 1980, **22**, 29 (*luminescence*)

Cooper, J.A. *et al*, *Inorg. Chim. Acta*, 1984, **92**, 23 (*synth, uv*)

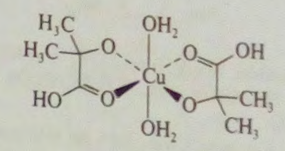
IC-006137

$C_8H_{18}CuO_8$

Diaquabis(2-hydroxy-2-methylpropanoato)copper

Diaquobis(2-*hydroxy*-2-*methylpropionato*)*copper*(II)

[22239-88-9]



M 305.7

Interatomic distances: Cu—OH_2 256, Cu—$OC(CH_3)_2$ 201, Cu—OCO 189 pm. Cryst.

Prout, C.K. *et al*, *J. Chem. Soc. A*, 1968, 2791 (*cryst struct, synth*)

IC-006138

$C_8H_{18}F_3O_8P_2Rh$

Trifluoroacetatobis(trimethyl phosphite)rhodium(*I*), 10CI

Bis(*trimethyl phosphite*)*rhodium*(I) *trifluoroacetate*

[71694-75-2]

$[(MeO)_3P]_2RhOOCCF_3$

M 464.0

Orange needles. Sol. toluene.

Sivak, A.J. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 4878 (*synth, pmr, P-31 nmr*)

IC-006139

$C_8H_{18}FeI_2O_2P_2$

Dicarbonyldiiodobis(trimethylphosphine)iron, 9CI, 8CI

[59460-91-2]

As Dibromodicarbonylbis(trimethylphosphine)iron, IC-006117 with

X = I

M 517.8

ab*-dicarbonyl-*df*-diiodo-*ce*-diphosphine-*form [62075-71-2]

cis,cis,trans-*form*

Deep-brown cryst. Mp 193°. μ = 3.9 D.

ab*-dicarbonyl-*ce*-diiodo-*df*-diphosphine-*form [15691-74-4]

di-trans,cis-*form*

Cryst., stable in air. Insol. nonpolar solvs. Dec. before melting. Transforms slowly in THF soln. to *cis,cis,trans*-form.

af*-dicarbonyl-*bd*-diiodo-*ce*-diphosphine-*form [51819-67-1]

di-trans,trans-*form*

Cryst. Dec. before melting.

Bancroft, G.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2103 (*mössbauer, ir, synth*)

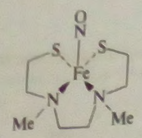
Pankowski, M. *et al*, *J. Organomet. Chem.*, 1977, **125**, 231 (*synth, ir, nmr*)

IC-006140

$C_8H_{18}FeN_3OS_2$

[[2,2'-[1,2-Ethanediylbis(methylimino)]bis[ethanethiolato]](2−)-N,N',S,S']nitrosyliron, 10CI

[64175-42-4]



M 292.2

Square pyramidal. Synth. from L_2Fe_2 + (NO)PF_6 or from L_2Fe_2 + NO. Green cryst. (CH_2Cl_2/Et_2O). Sol. CH_2Cl_2; insol. Et_2O.

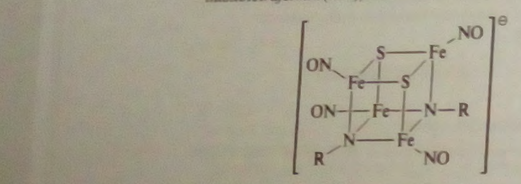
Karlin, K.D. *et al, Inorg. Chem.*, 1977, **16**, 3262 (*synth, struct, uv, ir*)

IC-006141

$C_8H_{18}Fe_4N_6O_4S_2^{\ominus}$

Bis(μ_3-*tert*-butylimido)bis(μ_3-sulfido)tetrakis(nitrosylferrate)(1−)

Bis[μ_3-[2-methyl-2-propanaminato(2−)]]tetranitrosyldi-μ_3-thioxotetraferrate(1−), 9CI



R = $C(CH_3)_3$

M 549.7 (ion)

Struct. is similar to parent neutral compd., but with longer Fe—Fe distances within the Fe_2N_2 and Fe_2S_2 units. Obt. by reduction of Bis[μ_3-[2-methyl-2-propanaminato(2−)]] tetranitrosyldi-μ_3-thioxotetrairon, IC-006142 with Na/Hg.

[Bis(triphenylphosphine)]iminium(1+) salt: [80399-52-6]. Black plate-like cryst. (THF/heptane).

Chu, C.T.-W. *et al, J. Am. Chem. Soc.*, 1982, **104**, 737 (*synth, struct*)

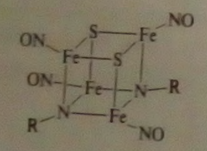
IC-006142

$C_8H_{18}Fe_4N_6O_4S_2$

Bis[μ_3-[2-methyl-2-propanaminato(2−)]]tetranitrosyldi-μ_3-thioxotetrairon, 9CI

Bis(μ_3-tert-butylimido)bis(μ_3-sulfido)tetrakis(nitrosyliron)

[53276-79-2]



R = $C(CH_3)_3$

M 549.7

Has cubane-like struct. Cryst. Diamagnetic.

Gall, R.S. *et al, J. Am. Chem. Soc.*, 1974, **96**, 4019 (*synth, cryst struct, ir, pmr*)

Sedney, D. *et al, Inorg. Chim. Acta*, 1979, **34**, 231 (*mössbauer*)

Chu, C.T.-W. *et al, J. Am. Chem. Soc.*, 1982, **104**, 737 (*synth, cryst struct*)

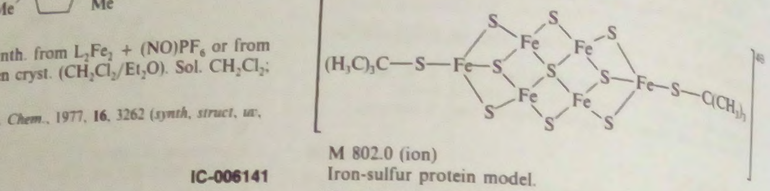
Butler, A.R. *et al, Adv. Inorg. Chem. Radiochem.*, 1988, **32**, 335 (*rev*)

$C_8H_{18}Fe_6S_{11}^{4\ominus}$

IC-006143

Bis(2-methyl-2-propanethiolato)hexa-μ-thioxodi-μ_3-thioxo-μ_4-thioxohexaferrate(4−), 10CI

Bis(tert-butylthio)hexa-μ-sulfidodi-μ_3-sulfido-μ_4-sulfidohexaferrate(4−)



M 802.0 (ion)

Iron-sulfur protein model.

Tetra-Li salt: Synth. from $FeCl_3$ + Li_2S + $LiSC(CH_3)_3$ in MeOH with LiOMe. Dark brown.

Tetrakis-benzyltrimethylammonium salt: [80976-82-5]. Black cryst. + 1MeOH (DMSO/MeOH). Sol. DMSO

Christou, G. *et al, J. Am. Chem. Soc.*, 1981, **103**, 6269 (*synth, struct, uv, mössbauer*)

Christou, G. *et al, Inorg. Chem.*, 1982, **21**, 3518 (*synth, struct, electrochem*)

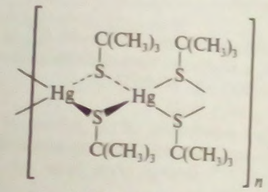
$C_8H_{18}HgS_2$

IC-006144

Bis(*tert*-butylthio)mercury(*II*)

Bis(2-methylpropane-2-thiolato)mercury, 9CI

[3374-16-1]



Solid-state form

M 378.9

Polymeric in solid state; monomeric in Py or in $CHCl_3$. Needles ($CHCl_3$/EtOH). Insol. H_2O, Et_2O, EtOH, MeOH; sol. cold $CHBr_3$; sol. hot Py, toluene, $CHCl_3$, CCl_4, $ClCH_2CH_2Cl$; sl. sol. $MeNO_2$, 2-propanol. Mp 159-160°, 165°. Bp 135° *in vacuo*.

[64762-07-8]

Rheinboldt, H. *et al, J. Prakt. Chem.*, 1932, **134**, 257 (*synth*)
Kunchur, N.F., *Nature (London)*, 1964, **204**, 468 (*cryst struct*)
Biscarini, P. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 2140 (*ir, raman*)
Canty, A.J. *et al, Inorg. Chim. Acta*, 1976, **20**, 161; 1977, **24**, 109 (*ir, raman, synth, pmr*)
Aycock, D.F. *et al, J. Org. Chem.*, 1979, **44**, 569 (*synth*)
Biscarini, P. *et al, Inorg. Chim. Acta*, 1981, **50**, 243 (*pe*)
Dean, P.A.W. *et al, Inorg. Chem.*, 1987, **26**, 4245 (*Hg-199 nmr*)

$C_8H_{18}MnO_2$

IC-006145

Di-*tert*-butoxymanganese(*II*)

Bis(2-methyl-2-propanolato)manganese. tert-*Butanol. manganese(2+) salt*

[69887-91-8]

$Mn[OC(CH_3)_3]_2$

M 201.1

Struct. not known. Synth. from $Mn[N(SiMe_3)_2]_2$.THF and *tert*-butanol in pentane. Pale rose solid, oxygen sensitive. Insol. pentane, C_6H_6, MeCN, THF.

Py complex: $C_{13}H_{23}MnNO_2$ M 280.2
Yellow cryst.

Horvath, B. *et al, Z. Anorg. Allg. Chem.*, 1979, **449**, 41 (*synth, reflectance*)

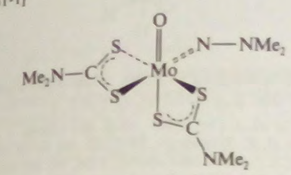
IC-006146

$C_8H_{18}MoN_4OS_4$

Bis(dimethyldithiocarbamato)[*N,N*-dimethylhydrazido(2−)-*N*']oxomolybdenum(*VI*)

Bis(dimethylcarbamodithioato-S,S')[1,1-dimethylhydrazinato(2−)-N^2]oxomolybdenum(VI), *1ICI, 10CI*

[53540-31-1]



M 410.4

Octahedral. Synth. from Me_2NNH_2 + $MoO_2(S_2CNMe_2)_2$. Pink, air-stable cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2, 1,2-dichloroethane. Mp 220-222°. Reacts with acids HX to give $MoX_2(NNMe_2)(S_2CNMe_2)_2$ (X = Cl, Br, SPh etc.). Ir ν_{MoO} 889 cm^{-1} (nujol).

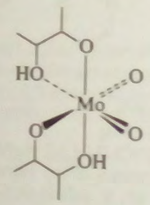
Bishop, M.W. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1600 (*cryst struct, synth, ir, pmr*)
Crichton, B.A.L. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 419 (*props*)
Chatt, J. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 1041 (*reactions*)

IC-006147

$C_8H_{18}MoO_6$

Bis(2,3-butanediolato-O,O')dioxomolybdenum(*VI*), 11CI, 10CI, 9CI

[59269-02-2]



M 306.1

cis-Octahedral.

Butane-2,3-diol complex: [71830-09-6]. Cryst. (MeCN). Mp 89°.

Butcher, R.J. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 356; 1979, 668 (*synth, cryst struct*)
Tung, K. *et al, Transition Met. Chem.*, 1986, **11**, 95 (*use*)

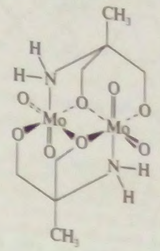
IC-006148

$C_8H_{18}Mo_2N_2O_8$

Bis[μ-[2-amino-2-methyl-1,3-propanediolato(2−)-$N,O:O'$]]tetraoxodimolybdenum(*VI*), 12CI

Bis[[μ-(2-amino-2-methyl-1,3-propanediolato(2−)-N,O:O')]dioxomolybdenum(VI)]

[107596-02-1]



M 462.1

Struct. consists of two tripod ligands bridging both Mo atoms. Interatomic distances: Mo—O_{bridge} 214.2, 221.3, Mo...Mo 355 pm. Colourless needles + 2DMSO.

McKee, V. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 523 (*cryst struct, synth*)

IC-006149

$C_8H_{18}N_2NiP_2$

Bis(cyano-*C*)bis(trimethylphosphine)nickel(*II*), 9CI

Bis(trimethylphosphine)dicyanonickel(II)

[20523-09-5]

$Ni(CN)_2(PMe_3)_2$

M 262.8

trans-Square planar. Yellow solid (Me_2CO/Et_2O). Sol. Me_2CO, CH_2Cl_2. Mp 235-240°. Diamagnetic. Ir_{CN} 2106 cm^{-1}. μ_{eff} = 0.37μ_B (298K).

[38889-86-0]

Merle, A. *et al, J. Coord. Chem.*, 1974, **3**, 199 (*synth*)
Dartiguenave, M. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 22531 (*pmr*)
Lukosius, T.J. *et al, Inorg. Chem.*, 1975, **14**, 1922, 1926 (*synth, ir, uv-vis, pmr*)
Meier, P. *et al, J. Am. Chem. Soc.*, 1976, **98**, 6402 (*P-31 nmr*)

IC-006150

$C_8H_{18}N_2NiP_2S_2$

Bis(thiocyanato-*N*)bis(trimethylphosphine)nickel(*II*)

[39046-04-3]

$Ni(NCS)_2(PMe_3)_2$

M 327.0

trans-Square planar. Brick-red, or orange-yellow solid. Sol. CH_2Cl_2. Mp 149-150°. Diamagnetic. μ_{eff} = 0.37μ_B. Ir ν_{CN} 2100, 2050 cm^{-1}.

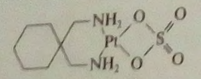
Beg, M.A.A. *et al, Can. J. Chem.*, 1961, **39**, 595 (*synth, uv-vis*)
Jensen, K.A. *et al, Acta Chem. Scand.*, 1968, **26**, 1044 (*synth*)
Merle, A. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1971, **272**, 1956 (*synth, ir, raman*)
Merle, A. *et al, J. Mol. Struct.*, 1972, **13**, 413 (*synth, uv-vis, ir, raman*)

$C_8H_{18}N_2O_4PtS$ IC-006151

Spiroplatin, BAN, INN, USAN

(1,1-Cyclohexanedimethanamine-N,N')[sulfato(2−)-O,O']platinum, 9CI. 1,1-Cyclohexanebis(methylamine)(sulfato)platinum. NSC 311056, TNO 6

[74790-08-2]



M 433.3

Antineoplastic agent. V. pale yellow cryst.

U.K. Pat., 2 024 823, (1980); *CA*, **93**, 114040p (*synth, tox, pharmacol*)
Vermorken, J.B. *et al, Dev. Oncol.*, 1984, **17**, 330 (*pharmacol*)
Vermorken, J.B. *et al, Recent Adv. Chemother., Proc. Int. Congr. Chemother., 14th, 1985*, (Anticancer Sect. 1), 1985, 96 (*rev, pharmacol*)
Barnard, C.F.J. *et al, Chem. Ber.*, 1986, **22**, 1001 (*rev*)
Van Hennik, M.B. *et al, Cancer Res.*, 1987, **47**, 6297 (*pharmacokinetics*)
Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 18684.

$C_8H_{18}N_2O_5S_5U$ IC-006152

Tris(dimethyl sulfoxide)bis(isothiocyanato)dioxouranium(*VI*)

Uranyl isothiocyanate tris(dimethyl sulfoxide)

[19600-05-6]

$$UO_2(NCS)_2(O{=}SMe_2)_3$$

M 620.6

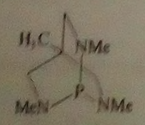
Air-stable yellow prisms (MeOH). Sol. MeOH. Mp 105-120°. Bp 270° dec. Ir ν_{CN} 2062, 2042, $\nu_{O=S=O}$ 914 cm^{-1}.

Shchelokov, R.N. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1966, **166-168**, 640 (*synth, ir*)
Shchelokov, R.N. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 660

$C_8H_{18}N_3P$ IC-006153

2,4,6,7-Tetramethyl-2,6,7-triaza-1-phosphabicyclo[2.2.2]octane, 9CI, 8CI

[14418-26-9]



M 187.2

Ligand for metals of Group VI B. Liq. Bp_{10} 82-86°.

1-Oxide: [15199-21-9]
$C_8H_{18}N_3OP$ M 203.2
Cryst. (EtOH). Mp 97-99°.

1-Sulfide: [15199-22-1]
$C_8H_{18}N_3PS$ M 219.2
Cryst. Mp 92.5-94.5°. Subl. 50° *in vacuo*.

1-Selenide: [68378-99-4]
$C_8H_{18}N_3PSe$ M 266.1
Solid. Mp 118-120°. $Subl._{0.01}$ 60°.

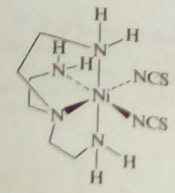
Laste, B.L. *et al, Inorg. Chem.*, 1967, **6**, 173 (*synth, derivs, pmr*)
Mosbo, J.A. *et al, J. Magn. Reson.*, 1972, **8**, 243 (*pmr, complexes*)
Claridy, J.C. *et al, Phosphorus*, 1974, **4**, 133 (*synth, oxide, cryst struct*)
Cowley, A.H. *et al, Inorg. Chem.*, 1977, **16**, 854; 1982, **21**, 543 (*pr*)
Kroshefsky, R.D. *et al, Inorg. Chem.*, 1979, **18**, 469 (*selenide, synth, P-31 nmr*)
Kroshefsky, R.D. *et al, Phosphorus Sulfur*, 1979, **6**, 391, 397 (*ir, cmr, derivs*)
Volcko, E.J. *et al, Phosphorus Sulfur*, 1984, **21**, 111 (*synth*)

$C_8H_{18}N_6NiS_2$ IC-006154

Diisothiocyanato[tris(2-aminoethyl)amine]nickel

[N,N-Bis(2-aminoethyl)-1,2-ethanediamine-N,N',N°,N'']bis(thiocyanato-N)nickel, 9CI. [4-(2-Aminoethyl)diethylenetriamine]bis(isothiocyanato)nickel(II), 8CI.

[15347-43-0]



M 321.0

Approx. *cis*-octahedral complex. Blue-violet cryst. (H_2O) Mp 285° dec. $\mu_{eff} = 3.19\mu_B$ (2.82K).

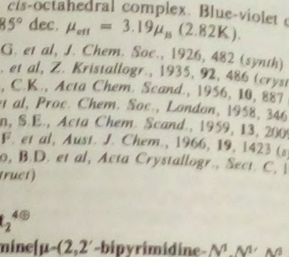
Mann, F.G. *et al, J. Chem. Soc.*, 1926, 482 (*synth*)
Cox, E.G. *et al, Z. Kristallogr.*, 1935, **92**, 486 (*cryst struct*)
Jorgensen, C.K., *Acta Chem. Scand.*, 1956, **10**, 887 (*uv*)
Hall, D. *et al, Proc. Chem. Soc., London*, 1958, 346 (*cryst struct*)
Rasmussen, S.E., *Acta Chem. Scand.*, 1959, **13**, 2009 (*synth, struct*)
Curtis, N.F. *et al, Aust. J. Chem.*, 1966, **19**, 1423 (*synth, ir*)
Santarsiero, B.D. *et al, Acta Crystallogr., Sect. C*, 1983, **39**, 1216 (*cryst struct*)

$C_8H_{18}N_8Pt_2^{4\oplus}$ IC-006155

Tetraammine[μ-(2,2'-bipyrimidine-$N^1,N^{1'},N^3,N^{3'}$)]diplatinum(*II*)(4+), 10Cl

Tetraammine(2,2'-bipyrimidyl)diplatinum(II)

[69063-62-3]



M 616.4 (ion)

Tentative struct. shown.

Tetranitrate: [69063-63-4].
Synth. from *cis*-$[PtCl_2(NH_3)_2]$, $AgNO_3$ and 2,2'-bipyrimidine. As tetrahydrate: brown soln. in H_2O, solid readily forms an oil. V. sol. H_2O. Dec. readily in presence of strong ligands.

Kiernan, P.M. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 1127 (*synth, props, ir*)

$C_8H_{18}NiO_2P_2$ IC-006156

Dicarbonylbis(trimethylphosphine)nickel, 9CI, 8CI

Bis(trimethylphosphine)dicarbonylnickel

[16787-34-1]

$$Ni(CO)_2(PMe_3)_2$$

M 266.8

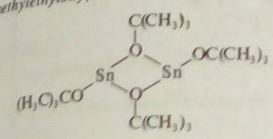
Catalyst for hydrosilylation of isoprene and dimethylbutadiene. Cryst. (pentane or MeOH).

Bignorgne, M. *et al, Bull. Soc. Chim. Fr.*, 1960, 1986 (*synth, ir*)
Bouquet, G. *et al, J. Mol. Struct.*, 1968, **1**, 211 (*ir, raman*)
Mathieu, R. *et al, Inorg. Chem.*, 1970, **9**, 2030 (*nmr*)
Koenig, M.F. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 1693 (*raman*)
Grobe, J. *et al, Z. Naturforsch., B*, 1981, **36**, 8 (*synth*)
Bochmann, M. *et al, J. Organomet. Chem.*, 1987, **332**, 361 (*synth*)

$C_8H_{18}O_2Sn$ IC-006157

Di-*tert*-butoxytin

Di-tert-butoxystannylene. Tin(II) tert-butoxide. Bis(1,1-dimethylethyloxy)tin



dimer

M 264.9

Dimeric in gas phase and in soln.

Dimer: [84913-53-1]. *Di-μ-tert-butoxydi-tert-butoxyditin. Bis[μ-(2-methyl-2-propanolato)]bis(2-methyl-2-propanolato)ditin, 11CI*
$C_{16}H_{36}O_4Sn_2$ M 529.8
Colourless cubes (toluene). Sol. C_6H_6. $Subl._{0.001}$ 60°.

Veith, M. *et al, J. Organomet. Chem.*, 1983, **246**, 219.
Fjeldberg, T. *et al, J. Chem. Soc., Chem. Commun.*, 1985, 939 (*synth, ed, Sn-119 nmr*)

$C_8H_{18}S_2Sn$ IC-006158

Bis(*tert*-butylthio)tin

Bis(tert-butylthio)stannylene

$$(H_3C)_3CSSnSC(CH_3)_3$$

M 297.0

Dimeric in C_6H_6. Yellow needles (toluene). Sol. C_6H_6. Mp 134° dec.

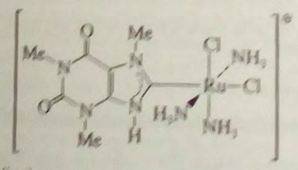
Dimer:
$C_{16}H_{36}S_4Sn_2$ M 594.1

du Mont, W.W. *et al, Chem. Ber.*, 1985, **118**, 1045 (*synth, ir, raman, pmr, cmr, Sn-119 nmr*)

$C_8H_{19}Cl_2N_7O_2Ru^{\oplus}$ IC-006159

Triammine dichloro(1,2,3,6,7,9-hexahydro-1,3,7-trimethyl-2,6-dioxo-8*H*-purin-8-ylidene)ruthenium(1+), 9CI

Triammine dichloro(1,3,7-trimethylxanthine)ruthenium(III)(1+). Triammine(caffeine)dichlororuthenium(III)(1+)



M 417.2 (ion)

mer, cis-Octahedral with Ru—C 203, Ru—$Cl_{trans\,to\,N}$ 235, Ru—$Cl_{trans\,to\,C}$ 242.7, Ru—$N_{trans\,to\,N}$ 211, Ru—$N_{trans\,to\,C}$ 207 pm.

Chloride: [64601-01-0].
Synth. from Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 + caffeine, followed by aerial oxidation and ion-exchange chromatog. Purple cryst. (1*M* HCl/EtOH).

[55208-41-8]

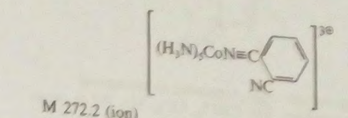
Krentzien, H.J. *et al, Bioinorg. Chem.*, 1975, **4**, 143 (*cryst struct*)
Clarke, M.J. *et al, J. Am. Chem. Soc.*, 1975, **97**, 1397 (*synth, uv*)

$C_8H_{19}CoN_7^{3\oplus}$ IC-006160

Pentaammine(1,2-dicyanobenzene)cobalt(*III*)(3+)

Pentammine(1,2-phenylenedicarbonitrile-N)cobalt(III)(3+)

[53739-00-7]



M 272.2 (ion)

Reaction of coordinated C≡N gives Pentaammine(2-cyanobenzamidato-N^1)cobalt(*III*)(2+). IC-006205.

Tri-perchlorate: Yellow solid. Sol. DMSO, H_2O.
▷ Potentially explosive.

Balabura, R.J., *Can. J. Chem.*, 1974, **52**, 1762 (*synth, ir, uv*)
Balabura, R.J. *et al, Inorg. Chem.*, 1979, **18**, 937; 1981, **20**, 4159 (*synth, pmr, kinetics*)

$C_8H_{20}AlO_2^{\ominus}$ IC-006161

Bis(*tert*-butanolato)dihydroaluminate(1−)

Dihydrobis(2-methyl-2-propanolato)aluminate(1−). Di-tert-butoxydihydroaluminate(1−)

$$AlH_2[OC(CH_3)_3]_2^{\ominus}$$

M 175.2 (ion)

Li salt: [24315-46-6].
Synth. from $LiAlH_4$ and Bu^{t}OH in THF. Selective reducing agent for ketones. White moisture-sensitive solid (Et_2O).

Abdel Kader, M.H., *Tetrahedron Lett.*, 1969, 2301 (*pmr*)
Abdel Kader, M.H., *Chem. Ber.*, 1970, **103**, 1225 (*synth, ir*)
Fusek, J. *et al, Collect. Czech. Chem. Commun.*, 1976, **41**, 187 (*ir*)
Šimon, O. *et al, Acta Chem. Scand., Ser. A*, 1977, **31**, 391 (*analogues*)
Turova, N.Ya., *Inorg. Chim. Acta*, 1977, **21**, 157
Turova, N.Ya., *Zh. Obshch. Khim.*, 1977, **47**, 1238
Horne, D.A. *et al, J. Am. Chem. Soc.*, 1980, **102**, 6911 (*synth, pmr, cmr, Li-7, Al-27 nmr*)
McMahon, R. *et al, J. Org. Chem.*, 1983, **48**, 99 (*use*)

$C_8H_{20}AsClN_2$ IC-006162

Chlorobis(diethylamino)arsine, 8CI

Tetraethylarsenodiamidous chloride, 9CI. Chlorobis(diethylamido)arsenic

[1734-99-2]

$$(Et_2N)_2AsCl$$

M 254.6

Liq. d_4^{20} 1.12. Bp_{12} 118-120°, $Bp_{0.1}$ 49-49°. n_D^{20} 1.5096.

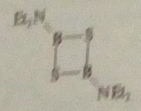
Kamai, G. *et al, Zh. Obshch. Khim.*, 1956, **26**, 126; *J. Gen. Chem. USSR (Engl. Transl.)*, 1956, **26**, 125 (*synth*)
Abel, E.W. *et al, J. Chem. Soc.*, 1965, 57 (*synth*)
McBeaerty, C.F. *et al, J. Organomet. Chem.*, 1968, **12**, 377 (*synth*)

$C_6H_{20}B_2N_2S_2$ IC-006163

2,4-Bis(diethylamino)-1,3,2,4-dithiadiboretane

N,N,N',N'-Tetraethyl-1,3,2,4-dithiadiboretane-2,4-diamine, 10Cl, 9Cl

[6105-36-8]



M 230.0

White, v. hygroscopic cryst. (pentane) as tetragonal tablets, air-sensitive. Sol. $CHCl_3$, CCl_4. Mp 70° *in vacuo*.

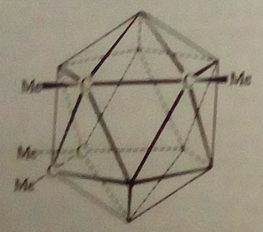
Forster, J.A. et al, Inorg. Chem., 1966, **5**, 164 (*synth, props, ir, pmr, B-11 nmr*)
Rivett, G.A., CA, 1976, **84**, 31231q (*struct*)
Bushnell, G.W. et al, Can. J. Chem., 1977, **55**, 3294 (*struct*)

$C_5H_{20}B_2$ IC-006164

C,C,C',C'-Tetramethyltetracarbadodecaborane(12), 10Cl, 9Cl

2,3,7,8-Tetramethyl-2,3,7,8-tetracarbadodecaborane(12)

[58815-26-2]



M 202.7

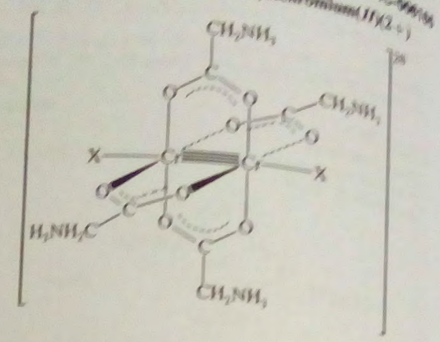
Exists in two isomeric forms which are in equilibrium in soln.; formally *nido*-type. Air stable colourless cryst. (hexane). Sol. CCl_4, $CHCl_3$, THF, MeCN, CH_2Cl_2, EtOH, C_6H_6. Mp 138°.

[54887-54-1]

Maxwell, W.M. et al, Inorg. Chem., 1976, **15**, 1343; 1977, **16**, 3094 (*synth, ir, pmr, B-11 nmr, ms*)
Freyberg, D.P. et al, Inorg. Chem., 1977, **16**, 1847 (*cryst struct*)
Hosmane, N.S. et al, Inorg. Chem., 1980, **19**, 3482 (*synth*)
Grimes, R.N., Adv. Inorg. Chem. Radiochem., 1983, **26**, 55 (*rev, bibl*)

$C_6H_{20}Br_2Cr_2N_4O_8^{2\oplus}$ IC-006165

Dibromotetrakis(μ-glycine-*O,O'*)dichromium(*II*)(2+)



X = Br

M 564.0 (ion)

Dinuclear $Cr_2^{4\oplus}$ unit bridged by glycine zwitterions; Cr—Cr 251.3, Cr—Br 273.6pm.

Dibromide: [92126-99-3].

Red-purple cryst. + $4H_2O$. Dec. in H_2O. $\mu_{eff} = 0.7\mu_B$ (293K).

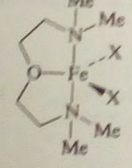
Herzog, S. et al, Z. Anorg. Allg. Chem., 1967, **351**, 237 (*synth, props*)
Ardon, M. et al, Inorg. Chem., 1984, **23**, 3450 (*cryst struct*)

$C_6H_{20}Br_2FeN_2O$ IC-006166

Dibromo[bis(2-dimethylaminoethyl) ether]iron(*II*)

Dibromo[2,2'-oxybis[N,N'-dimethylethanamine]]iron(II)

[15079-42-2]



X =Br

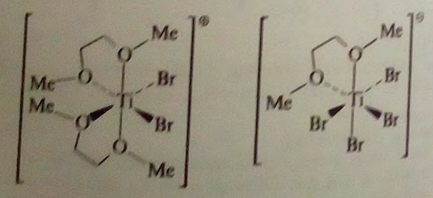
M 375.9

Trigonal bipyramidal Fe(*II*). Synth. from $FeBr_2$ + ligand in 1-butanol. Pale pink; oxidises in air. $\mu_{eff} = 5.26\mu_B$ (295K).

Ciampolini, M. et al, Inorg. Chem., 1967, **6**, 445 (*synth, se, magnetism*)

$C_8H_{20}Br_2O_4Ti^{\oplus}$ IC-006167

Dibromobis(1,2-dimethoxyethane)titanium(*III*)(1+), 8Cl



tetrabromo(dimethoxyethane)titanate salt

M 387.9 (ion)

It is suggested that many $TiX_3.5L$ spp. may have similar ionic structures.

Tetrabromo(1,2-dimethoxyethane)titanate(1−): [24692-58-8] Hexabromotris(1,2-dimethoxyethane)dititanium(III)

$C_{12}H_{30}Br_6O_6Ti_2$ M 845.5

Synth. by heating $TiBr_3$ in 1,2-dimethoxyethane under reflux. Green, air-sensitive solid. $\mu_{eff} = 1.67\mu_B$ per titanium.

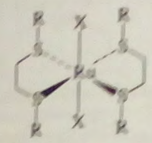
Fowles, G.W.A. et al, J. Inorg. Nucl. Chem., 1967, **29**, 2365 (*synth, magnetism, se, ir*)
Fowles, G.W.A. et al, J. Inorg. Nucl. Chem., 1969, **31**, 657 (*cryst struct*)

$C_6H_{20}Br_2RuS_4$, IC-006168

Bis(1,2-bis(methylthio)ethane-*S,S'*)dibromoruthenium(*II*), 9Cl

Dibromobis(1,2,5-dithiahexane)ruthenium(II)

[32648-27-4]



R = Me , X = Br

M 505.3

trans-Octahedral. Prepd. by treating $RuBr_3.xH_2O$ in boiling 2-methoxyethanol with $MeSCH_2CH_2SMe$. Lilac cryst. (butanol). Mp > 250°.

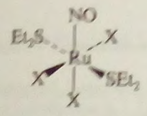
Chatt, J. et al, J. Chem. Soc. A, 1971, 1380 (*synth, ir, pmr, se*)
Gulliver, D.J. et al, Inorg. Chim. Acta, 1983, **69**, 25 (*pmr*)

$C_6H_{20}Br_3NORuS_2$ IC-006169

Tribromobis(diethyl sulfide)(nitrosyl)ruthenium

Tribromo(nitrosyl)bis[1,1'-thiobis[ethane]]ruthenium, 9Cl

[61567-06-4]



X = Br

M 551.1

Single *mer,trans*-octahedral isomer obsd. Prepd. by treating an NO-saturated EtOH soln. of $RuBr_3.xH_2O$ with SEt_2. Red solid; oxidised in $CHCl_3$ soln. by air and sunlight to the novel diethylsulfoxide complex $(\mu\text{-Br})_2[Ru(NO)(OSEt_2)Br_2]_2$. Ir ν_{NO} 1857; ν_{Ru-Br} 249, 229 cm^{-1}.

Ferguson, J.E. et al, Aust. J. Chem., 1976, **29**, 2159 (*synth, ir, se, pmr, cmr*)
Ferguson, J.E. et al, Inorg. Chem., 1976, **15**, 2270 (*reaction*)
Page, C.T. et al, Aust. J. Chem., 1983, **36**, 855 (*pmr*)
Coll, R.K. et al, Aust. J. Chem., 1986, **39**, 1161 (*photochem*)
Coll, R.K. et al, Inorg. Chem., 1987, **26**, 106 (*photochem*)

$C_6H_{20}Br_4P_2S_2$ IC-006170

Tetrabromobis(diethyl sulfide)diplatinum(*II*)

Tetrabromobis[μ-(1,1'-thiobisethane)]diplatinum, 9Cl

[21315-77-5]

X = Br

M 890.1

Cryst. struct. shows molecule to be S-bridged. Synth. from $Na_2PtCl_4.4H_2O$, NaBr and $PtBr_2(SEt_2)_2$. Yellow cryst. (purif. by continuous extraction with CH_2Cl_2). Mp 221-223°.

Sales, D.L. et al, J. Chem. Soc. A, 1968, 1852 (*cryst struct*)
Adams, D.M. et al, J. Chem. Soc. A, 1969, 588 (*ir*)
Goggin, P.L. et al, J. Chem. Soc., Dalton Trans., 1974, 576 (*synth*)

$C_8H_{20}CdO_8P_2$ IC-006171

Bis(*O,O*-diethyl phosphato-*O,O'*)cadmium(*II*)

Cadmium(II) diethyl phosphate

[17071-46-6]

$Cd[O_2P(OEt)_2]_2$

M 418.6

Solid state struct. comprises infinite chains of dimeric units containing 6-coordinate Cd. Needles (EtOH).

Minter, V.W. et al, Inorg. Chem., 1983, **22**, 1862 (*synth, cryst struct*)
Minter, V.W. et al, J. Am. Chem. Soc., 1985, **107**, 2177 (*CP-MAS nmr*)

$C_{10}H_{20}ClNbO_4$ IC-006172

Chlorotetraethoxyniobium(*V*), 11Cl

[6477-35-6]

$NbCl(OEt)_4$

M 308.6

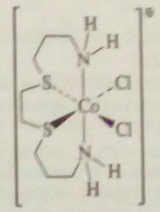
Struct. not known. Synth. from $NbCl_5$ and EtOH; or from $NbCl_5$ and diethyl sulfite in CCl_4. Colourless solid. Mp 104°.

Kolditz, L. et al, Z. Chem., 1965, **5**, 349 (*synth*)
Nisel'son, L.A. et al, Russ. J. Inorg. Chem. (Engl. Transl.), 1984, **29**, 1289 (*synth, ir*)

$C_8H_{26}Cl_2CoN_2S_2^{\oplus}$ IC-006173

Dichloro(1,10-diamino-4,7-dithiadecane)cobalt(*III*)(1+)

Dichloro[3,3'-(ethylenedithio)bis[propylamine]]cobalt(1+), 8Cl



cis-α-form

M 338.2 (ion)
Two *cis*-isomers were isolated and designated *cis*-α and *cis*-β.

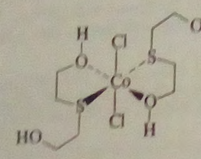
***cis*-α-form**
Perchlorate: [24717-60-0].
Blue cryst.
▷ Potentially explosive.

***cis*-β-form**
Perchlorate: Red-violet needles.

Bosnich, B. *et al, Inorg. Chem.*, 1969, **8**, 2567 (*synth, uv*)

IC-006174

$C_8H_{20}Cl_2CoO_4S_2$
Dichlorobis[2,2′-thiobis(ethanol)-*O,S*]cobalt(*II*), 10Cl
Dichlorobis(2,2′-thiodiethanol)cobalt(II)
[74779-08-1]



M 374.2
Octahedral. Pink cryst.

Ucliupa, M.R. *et al, Inorg. Chim. Acta*, 1980, **41**, 31 (*synth, cryst struct*)

IC-006175

$C_8H_{20}Cl_2CoS_4$
Dichlorobis(2,5-dithiahexane)cobalt(*II*)
Bis(2,5-dithiahexane)dichlorocobalt(II)

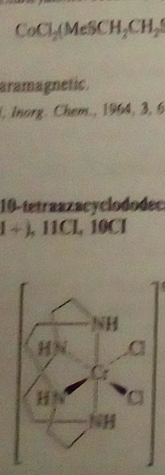
$CoCl_2(MeSCH_2CH_2SMe)_2$

M 374.3
Purple solid. Paramagnetic.

Carlin, R.L. *et al, Inorg. Chem.*, 1964, **3**, 611 (*synth, uv, magnetism*)

IC-006176

$C_8H_{20}Cl_2CrN_4^{\oplus}$
Dichloro(1,4,7,10-tetraazacyclododecane-N^1,N^4,N^7,N^{10}) chromium(*III*)(1+), 1ICl, 10Cl
[101009-52-3]



M 295.1 (ion)
Octahedral cation. *trans*-form unknown. Weak field aza ligand bound in strained manner.

***cis*-form**
With aq. $[NH_4]SCN$ gives *cis*-dithiocyanato-*N* deriv.

Chloride: [78804-39-4].
Synth. by refluxing $CrCl_3.6H_2O$ + macrocycle in EtOH in presence of activated Zn. Blue solid (HCl/EtOH). μ_{eff} = 3.6μ_B (298K).

Swisher, R.G. *et al, Inorg. Chem.*, 1981, **20**, 3947; 1986, **25**, 1320 (*uv-vis, synth, conductivity, ir, acid hydrolysis*)
Comp. Coord. Chem., Pergamon, Oxford, 1987, **3**, 922 (*rev*)

IC-006177

$C_8H_{20}Cl_2Cr_2N_4O_8^{2\oplus}$
Dichlorotetrakis(μ-glycine-*O,O′*)dichromium(*II*)(2+)
As Dibromotetrakis(μ-glycine-*O,O′*)dichromium(*II*)(2+), IC-006165 with

X = Cl

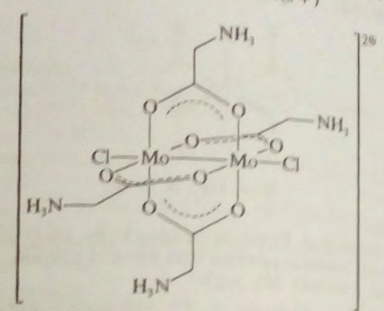
M 475.1 (ion)
Cr—Cr 252.4, Cr—Cl 258.1 pm.

Dichloride: [92127-00-9].
Purple cryst. + $3H_2O$. Dec. in H_2O.

Herzog, S. *et al, Z. Anorg. Allg. Chem.*, 1967, **351**, 237 (*synth, props*)
Ardon, M. *et al, Inorg. Chem.*, 1984, **23**, 3450 (*cryst struct*)

IC-006178

$C_8H_{20}Cl_2Mo_2N_4O_8^{2\oplus}$
Dichlorotetrakis[μ-(glycine-*O:O*)]dimolybdenum(*II*)(2+)
Tetrakis(glycine)dichlorodimolybdenum(2+)



M 563.0 (ion)

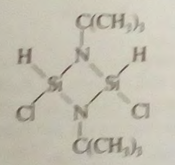
Chloride, 2½ hydrate: [69881-48-7].
Triclinic yellow cryst. Mo—Mo 210.8 pm.

Dichloride, trihydrate: [69881-47-6].
Monoclinic yellow cryst. Mo—Mo 211.2 pm.

Bino, A. *et al, Inorg. Chem.*, 1979, **18**, 1719 (*cryst struct*)

IC-006179

$C_8H_{20}Cl_2N_2Si_2$
1,3-Di-*tert*-butyl-2,4-dichloro-2,4-dihydrocyclo-2,4-disiletidine
1,3-Di-tert-butyl-2,4-dichloro-1,3-diaza-2,4-disilacylobutane
2,4-Dichloro-1,3-bis(1,1-dimethylethyl)cyclodisilazane



M 271.3
Exists as mixt. of isomers. Liq. $Bp_{0.01}$ 32°.

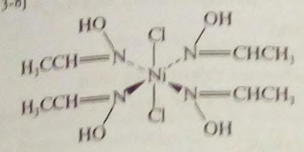
***cis*-form** [117367-34-7]

***trans*-form** [117367-44-9]

Bartholmei, S. *et al, Z. Anorg. Allg. Chem.*, 1988, **556**, 129 (*synth, props, cmr, ir, ms, nmr, pmr*)

IC-006180

$C_8H_{20}Cl_2N_4NiO_4$
Tetrakis(acetaldehyde oxime-*N*)dichloronickel(*II*), 9Cl
Tetrakis(acetaldoxime)dichloronickel(II)
[41930-73-8]



M 365.8
trans-Octahedral. Hygroscopic cryst. (EtOH/MeOH).
[36445-00-8]

Stone, M.E. *et al, J. Chem. Soc. A*, 1971, 3632 (*cryst struct*)
Stone, M.E. *et al, Can. J. Chem.*, 1973, **51**, 1260 (*synth, props, ir, uv*)
Tanaka, H. *et al, Bull. Chem. Soc. Jpn.*, 1977, **50**, 3259 (*synth, ir*)
Patel, N.A. *et al, Indian J. Chem., Sect. A*, 1980, **19**, 236 (*synth, cryst struct*)

IC-006181

$C_8H_{20}Cl_2N_4NiS_4$
Dichlorotetrakis(thioacetamide)nickel(*II*)
Dichlorotetrakis(ethanethioamide-S)nickel, 8Cl. Nickel(II) *chloride tetrakis(thioacetamide)*
[19621-53-5]

$NiCl_2[S{=}C(NH_2)CH_3]_4$

M 430.1
trans-Octahedral. Blue cryst. Paramagnetic.

Flint, C.D. *et al, J. Chem. Soc. A*, 1968, 750 (*synth, ir, uv*)
Girling, R.L. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 2640 (*cryst struct*)
Chatterjee, K.K., *Inorg. Chim. Acta*, 1972, **6**, 8 (*uv, magnetism*)

IC-006182

$C_8H_{20}Cl_2OP_2S_2V$
Dichlorooxo(tetraethyldiphosphine-1,2-disulfide-*S,S′*) vanadium(*IV*), 11Cl
[80849-11-2]

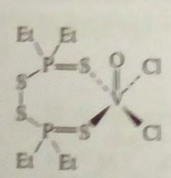
$VOCl_2[Et_2P(S)P(S)Et_2]$

M 380.1
Synth. by adding $VOCl_3$ in $CHCl_3$ to the ligand in $CHCl_3$ under reflux. Green air- and moisture-sensitive solid. Sol. polar solvs. Paramagnetic, g 1.990, Ir $\nu_{V=O}$ 995 cm^{-1}.

Cuadrado, I. *et al, Transition Met. Chem.*, 1981, **6**, 329 (*synth, ir, uv-vis, esr*)

IC-006183

$C_8H_{20}Cl_2OP_2S_4V$
Dichloro[dithiobis[diethylphosphine sulfide]] oxovanadium(*IV*), 11Cl
[90100-01-9]



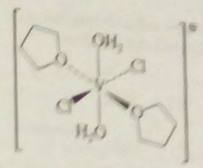
M 444.3

Square pyramidal. Synth. from $VOCl_3$ and the ligand in CH_2Cl_2. Sol. CCl_4. Ir $\nu_{V=O}$ 1000; ν_{S-S} 470 cm^{-1}. See also Dichlorooxo(tetraethyldiphosphine-1,2-disulfide-*S,S′*) vanadium(*IV*), IC-006182.

Cuadrado, I. *et al, Transition Met. Chem.*, 1984, **9**, 96 (*synth, uv-vis, ir, raman, esr*)

IC-006184

$C_8H_{20}Cl_2O_4V^{\oplus}$
Diaquadichlorobis(tetrahydrofuran)vanadium(*III*)(1+), 1ICl



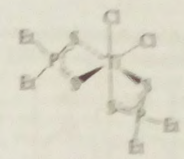
M 302.0 (ion)
trans-Octahedral cation.

Trichloro(tetrahydrofuran)zincate(1−): [93590-30-6].
$C_{12}H_{28}Cl_5O_5VZn$ M 545.9
Hydrolysis product formed during recryst. of $VCl_3.ZnCl_2.5THF$ from THF. Green cryst. + 1THF.

Folting, K. *et al, Inorg. Chem.*, 1984, **23**, 4589 (*synth, cryst struct*)

IC-006185

$C_8H_{20}Cl_2P_2S_4Ti$
Dichlorobis(diethyldithiophosphinato)titanium(*IV*)
Dichlorobis(diethylphosphinodithioato-S,S′)titanium(IV), *10Cl*
[78240-82-1]

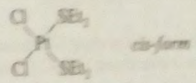


M 425.2
Synth. by mixing $TiCl_4$ with $Et_2P(S)SH$ in Me_4SiCl at 40-50°. Moisture-sensitive, red solid. Sol. CH_2Cl_2, C_6H_6. Mp 139.5-140°.

Kuchen, W. *et al, Z. Anorg. Allg. Chem.*, 1981, **472**, 110 (*cryst struct, synth, pmr, P-31 nmr, ir*)

IC-006186

$C_8H_{20}Cl_2PtS_2$
Dichlorobis(diethyl sulfide)platinum(*II*)
Dichlorobis(ethyl sulfide)platinum, 8Cl. Dichloro[1,1′-thiobis(ethane)]platinum, 9Cl. Bis(diethyl sulfide) dichloroplatinum
[14873-92-8]



cis-form

M 446.3
Synth. from $PtCl_2$ + SEt_2; use of excess SEt_2 gives *cis*-isomer. Synth. use by substitution of Cl. Catalyses crosslinking of siloxanes. Configuration inversion at S has been studied.

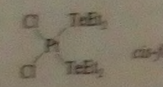
***cis*-form** [15442-57-6]
Pale green-yellow flakes (Me_2CO/pet. ether). Sol. polar org. solvs.; insol. hydrocarbons. Mp 107-108°.

trans-form [15557-84-5]
Bright yellow needles (EtOH aq.). Sol. org. solvs. including hydrocarbons. Mp 107-108° (95-100°).

Inorg. Synth., 1960, **6**, 211 (*synth*)
Allen, E.A. *et al. Spectrochim. Acta, Part A*, 1972, **28**, 725 (*ir, raman*)
McFarlane, W., *J. Chem. Soc., Dalton Trans.*, 1974, 324 (*P-31 nmr*)
Cross, R.J. *et al., J. Chem. Soc., Dalton Trans.*, 1976, 1130 (*pmr*)

$C_6H_{20}Cl_2PtTe_2$ IC-006187

Dichlorobis(diethyl telluride)platinum(*II*)
Dichlorobis(ethyl telluride)platinum
[53383-33-8]



cis-form

M 637.4
Square planar.

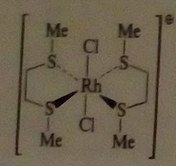
cis-form
Isom. to *trans*-form in C_6H_6 soln. Synth. from K_2PtCl_4 and Et_2Te. Brown-yellow cryst. (EtOH). Sol. C_6H_6. Mp 126-129°.

trans-form [59286-33-8]
Thought to be formed in C_6H_6 soln. by isom. of *cis*-form. Not isol.

Gmelin Handbook Inorg. Chem., Syst. No. 68, 1957, **D**, 341 (*synth, props*)
Cross, R.J. *et al., J. Chem. Soc., Dalton Trans.*, 1976, 382, 1150 (*props, ir, pmr*)

$C_8H_{20}Cl_2RhS_4^{\oplus}$ IC-006188

Bis[1,2-bis(methylthio)ethane]dichlororhodium(*III*)(1+)
Dichlorobis(2,5-dithiahexane)rhodium(III)(*1+*)



M 418.3 (ion)
trans-Octahedral.
Chloride: [19964-44-4].
Yellow solid. Spar. sol. MeCN, $MeNO_2$, EtOH.

Walton, R.A. *et al., J. Chem. Soc. A*, 1967, 1852 (*synth, ir*)

$C_8H_{20}Cl_2RuS_4$ IC-006189

Bis[1,2-bis(methylthio)ethane-*S,S'*]dichlororuthenium(*II*), 9Cl
Dichlorobis(2,5-dithiahexane-S,S')*ruthenium*(II)
[32801-98-2]

As Bis[1,2-bis(methylthio)ethane-*S,S'*] dibromoruthenium(*II*), IC-006168 with

R = Me, X = Cl

M 416.4
trans-Octahedral. Prepd. by treating '$RuCl_3.xH_2O$' in boiling 2-methoxyethanol with $MeSCH_2CH_2SMe$. Yellow solid. Mp >250°. Ir ν_{RuCl} 338 cm^{-1} (polythene).

Chatt, J. *et al., J. Chem. Soc. A*, 1971, 1380 (*synth, ir, pmr, uv*)
Gulliver, D.J. *et al., Inorg. Chim. Acta*, 1983, **69**, 25 (*pmr*)

$C_8H_{20}Cl_2RuS_4^{\oplus}$ IC-006190

Bis[1,2-bis(methylthio)ethane-*S,S'*]dichlororuthenium(III) (1+), 9Cl

$[RuCl_2]MeSCH_2CH_2SMe_2]^{\oplus}$

M 416.4 (ion)
Prob. *cis*-octahedral.
Tetraphenylborate: Yellow-green solid.

Rice, D.A. *et al., Inorg. Chim. Acta*, 1971, **5**, 683 (*synth*)

$C_8H_{20}Cl_3NORuS_2$ IC-006191

Trichlorobis(diethyl sulfide)(nitrosyl)ruthenium
Trichloro(nitrosyl)bis[1,1'-thiobis[ethane]]ruthenium, 9Cl
[61566-98-1]

As Tribromobis(diethyl sulfide)(nitrosyl)ruthenium, IC-006169 with

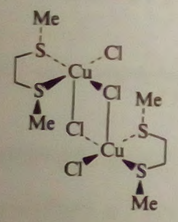
X = Cl

M 417.8
Single *mer,trans*-octahedral isomer obsd. Prepd. by treating an NO-saturated ethanolic soln. of $RuCl_3.xH_2O$ with SEt_2. Red-brown solid. Ir ν_{NO} 1868; ν_{RuCl} 356, 342, 334 cm^{-1}.

Fergusson, J.E. *et al., Aust. J. Chem.*, 1976, **29**, 2159 (*synth, ir, uv, pmr, cmr*)
Page, C.T. *et al., Aust. J. Chem.*, 1983, **36**, 855 (*pmr*)

$C_8H_{20}Cl_4Cu_2S_4$ IC-006192

Bis[1,2-bis(methylthio)ethane-*S,S'*]di-μ-chlorodichlorodicopper(*II*), 11Cl
Dichloro(2,5-dithiahexane)copper(II) *dimer*
[99727-67-0]



M 513.4
CuS_2Cl_2 is tetrahedrally distorted square planar. Dark green microcryst. (MeOH). Insol. MeOH.
Monomer:
$C_4H_{10}Cl_2CuS_2$ M 256.7

Hatfield, W.E. *et al., Inorg. Chem.*, 1986, **25**, 558 (*cryst struct, magnetism, uv, synth*)

$C_8H_{20}Cl_4Ir_2S_2^{2\ominus}$ IC-006193

Tetrachlorobis(diethyl sulfide)iridate(*III*)(1−)

$[IrCl_4(SEt_2)_2]^{\ominus}$

M 514.4 (ion)
trans-Config.
NH_4 salt: Orange cryst. Sol. EtOH.
Bis(pyridine)silver(1+) salt:
$C_{18}H_{30}AgCl_4IrN_2S_2$ M 780.4
Sol. Py. Mp 162°.

Kaufmann, G.B. *et al., Inorg. Chem.*, 1963, **2**, 1233 (*synth, uv, pmr*)

$C_6H_{20}Cl_4MoO_2$ IC-006194

Tetrachlorobis(diethyl ether)molybdenum(*IV*)
Tetrachlorobis[1,1'-oxybis(ethane)]molybdenum(IV), *11Cl*
Tetrachloromolybdenum(IV) *chloride bis(diethyl ether)*
[304111-56-4]

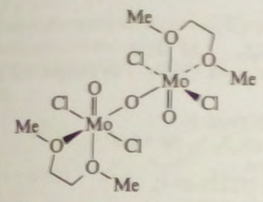
$MoCl_4(OEt_2)_2$

M 385.9
Synth. by treatment of $MoCl_5$ in Et_2O with norbornene. Used as catalyst for the metathesis of strained olefins. Starting material. Red-orange cryst. (Et_2O).

Castellani, L. *et al., Transition Met. Chem.*, 1985, **10**, 194 (*synth, props, use*)
Walborsky, E.C. *et al., Inorg. Chem.*, 1987, **26**, 1615 (*use*)

$C_6H_{20}Cl_4Mo_2O_7$ IC-006195

Tetrachlorobis(1,2-dimethoxyethane-*O,O'*)-μ-oxodioxodimolybdenum, 11Cl
μ-Oxobis[dichlorooxo[1,2-dimethoxyethane]]dimolybdenum(V)
[85343-07-3]



M 561.9
Mo coordination is significantly distorted from octahedral. Synth. from $MoCl_5$ in 1,2-dimethoxyethane acidified with formic or acetic acid. Air-sensitive olive-green cryst.

Kamenar, B. *et al, Inorg. Chim. Acta*, 1982, **65**, L245 (*cryst struct*)

$C_8H_{20}Cl_4N_2Nb^{\ominus}$ IC-006196

Tetrachlorobis(diethylamido)niobate(*V*)(1−)
Tetrachlorobis(N-*ethylethanaminato*)*niobate*(V)(*1−*), *11Cl*

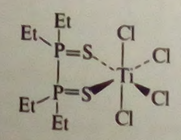
$[NbCl_4(NEt_2)_2]^{\ominus}$

M 378.9 (ion)
Octahedral, *cis* and *trans* isomers are said to be formed but not separately described.
Et_2NH_2 salt: [91321-02-7].
Synth from $NbCl_5$ and Et_2NH in C_6H_6.
[91383-87-8]

Ermakov, V.A. *et al, Koord. Khim.*, 1984, **10**, 817; *CA*, **101**, 102890m (*synth, ir, pmr*)

$C_8H_{20}Cl_4P_2S_2Ti$ IC-006197

Tetrachloro(tetraethyldiphosphine-1,2-disulfide) titanium(*IV*), 11Cl
[12080-85-2]



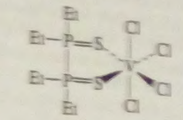
M 432.0

Synth. by slowly adding $TiCl_4$ in $CHCl_3$ to a soln. of $Et_4P_2S_2$ in $CHCl_3$. Orange, moisture-sensitive solid.

Cuadrado, I. *et al., Transition Met. Chem.*, 1981, **6**, 329 (*synth, ir*)

$C_8H_{20}Cl_4P_2S_2V$ IC-006198

Tetrachloro(tetraethyldiphosphine-1,2-disulfide-*S,S'*) vanadium(*IV*), 11Cl
Vanadium(IV) *chloride tetraethyldiphosphinedisulfide*
[80849-10-3]



M 435.0
Octahedral. Synth. by adding VCl_4 in $CHCl_3$ to a soln. of the ligand in $CHCl_3$. Green, air- and moisture-sensitive solid. Sol. Me_2CO. The methyl analogue is also known. $VOCl_3$ yields $VOCl_3L$. Paramagnetic, g 1.989 (solid), 1.987 (Me_2CO soln.).

Cuadrado, I. *et al, Transition Met. Chem.*, 1981, **6**, 329 (*synth, uv-vis, ir, esr*)

$C_8H_{20}Cl_4Pt_2S_2$ IC-006199

Tetrachlorobis(diethyl sulfide)diplatinum(*II*)
Tetrachlorobis[μ-[1,1'-thiobis(ethane)]]diplatinum, 9Cl
[23045-06-9]

As Tetrabromobis(diethyl sulfide)diplatinum(*II*), IC-006170 with

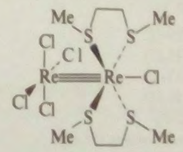
X = Cl

M 712.3
Shown by ir to have S-bridges, contrary to previous assignment of Cl-bridges. Synth. from *cis*-$(Et_2S)_2PtCl_2$ and Na_2PtCl_4 or from $(Et_2S)_2PtCl_2$ and $MeOSO_2F$. Bright yellow cryst. (purif. by continuous extraction with CH_2Cl_2). Pract. insol. all solvs. Mp 213-230° dec.
[75899-88-6]

Chatt, J. *et al, J. Chem. Soc.*, 1955, 2787 (*synth, props*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1969, 588 (*ir*)
Eaborn, C. *et al, J. Organomet. Chem.*, 1973, **55**, C68 (*synth*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 576 (*synth*)

$C_8H_{20}Cl_5Re_2S_4$ IC-006200

Bis[1,2-bis(methylthio)ethane]pentachlorodirhenium(*II,III*)
Pentachlorobis(2,5-dithiahexane)rhenium(II)*rhenium*(III)
[14973-60-5]



M 794.1
Re—Re 229.3 pm. Synth. from $(Bu_4N)_2Re_2Cl_8$ and dithiahexane in refluxing MeCN. Red-black dichroic cryst. Insol. Me_2CO, EtOH, MeCN, THF, $MeNO_2$.

Cotton, F.A. *et al, Inorg. Chem.*, 1967, **6**, 214 (*synth, ir*)
Bennett, M.J. *et al, Proc. R. Soc. London, A*, 1968, **303**, 175 (*cryst struct*)

IC-006201

$C_6H_{24}Cl_2Rh_2S_4$

Di-μ-chloro-tetrachlorobis(2,5-dithiahexane-*S,S'*)dirhodium(*III*)

Bis(μ-chloro)dichlorobis(2,5-dithiahexane)rhodium(III)

*As Di-μ-chlorotetrachlorobis(1,2-dithiocyanatoethane-*S,S'*)dirhodium(III), IC-005927 with*

X = Me6

M 465.0

Dimeric struct. is tentative. Synth. from $RhCl_3.3H_2O$ and 1,4-dithiane in EtOH. Pale yellow powder. V. spar. sol. MeCN, $MeNO_2$; insol. non-polar solvs.

Monomer: Trichloro(2,5-dithiahexane)rhodium(III)

$C_6H_{12}Cl_3RhS_2$ M 299.4

Watson, R.A. *et al. J. Chem. Soc. A*, 1967, 1852 (*synth., ir*)

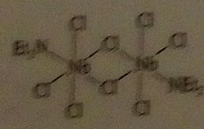
IC-006202

$C_8H_{20}Cl_4N_2Nb_2$

Di-μ-chloro-bis-tetrachlorobis(diethylamido)diniobium(*V*)

Di-μ-chloro-bis-tetrachlorobis(N-ethylethanaminato)diniobium(V), HCl. Tetrachloro(diethylamido)niobium(V) dimer

[84331-00-5]



M 613.6

Presumed bioctahedral; detailed geometry not established. Synth. from $NbCl_5$ and Et_2NH in C_6H_6.

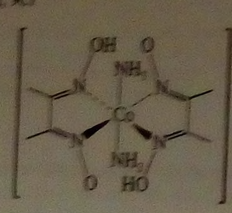
[81383-85-9]

Ermatov, V.A. *et al. Koord. Khim.*, 1984, **10**, 817; *CA*, **101**, 102890m (*synth., ir, pmr*)

$C_6H_{24}CoN_6O_4^{\oplus}$ IC-006203

Diamminebis(dimethylglyoximato)cobalt(*III*)(1+)

*Diammine(2,3-butanedione dioximato(1−)-*N,N'*)cobalt(1+), 9Cl*



M 323.2 (ion)

trans-form [35220-67-8]

Bromide: [72121-29-0].
Yellow cryst. (H_2O).

Chloride: [22452-51-3].
Brown plates (H_2O).

Nitrate: [59035-02-8].
Long orange-red needles (H_2O).

Thiocyanate: [30785-63-8].
Orange plates.

[14896-93-6, 18497-84-2]

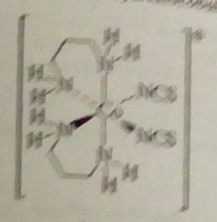
Nakatsuka, Y. *et al. Bull. Chem. Soc. Jpn.*, 1936, **11**, 49 (*synth*)
Akitsugu, N., *Bull. Chem. Soc. Jpn.*, 1955, **28**, 207 (*uv*)
Kunchur, N.R. *et al. Z. Anorg. Allg. Chem.*, 1959, **302**, 289 (*cryst struct, chloride, nitrate*)
Reichert, B.E. *et al. J. Chem. Soc., Chem. Commun.*, 1974, 177 (*Co-59 nmr*)

Elder, R.C. *et al. Acta Crystallogr., Sect. B*, 1980, **36**, 2692 (*cryst struct, nitrate, thiocyanate*)
Herzog, M.J. *et al. Inorg. Chem.*, 1980, **19**, 992 (*cryst struct, bromide*)

$C_6H_{24}CoN_8S_2^{\oplus}$ IC-006204

Bis(1,3-propanediamine-*N,N'*)bis(thiocyanato-*N*)cobalt(1+), 9Cl

Bis(1,3-diaminopropane)dithiocyanatocobalt(III)



cis-form

M 323.3 (ion)

Prepd. from the corresp. dichloro ion, by ligand substitution.

cis-form

Thiocyanate:
$C_8H_{20}CoN_6S_2$ M 381.4
Orange-red cryst. (H_2O). This compd. has been resolved.

trans-form

Chloride: [22229-02-3].
$C_6H_{20}ClCoN_6S_2$ M 358.8
Purple cryst.

Thiocyanate: [22229-03-4].
Deep-purple cryst.

[29962-40-1, 46752-66-3, 82025-96-7]

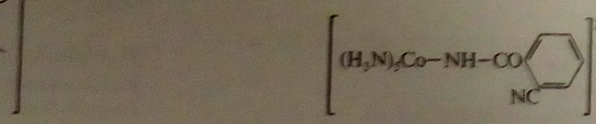
Kawaguchi, H. *et al. Bull. Chem. Soc. Jpn.*, 1969, **42**, 136; 1970, **43**, 2103 (*synth., ir, uv*)
Kanamore, K. *et al. Bull. Chem. Soc. Jpn.*, 1982, **55**, 1315 (*raman, ir*)

$C_6H_{20}CoN_7O^{2\oplus}$ IC-006205

Pentaammine(2-cyanobenzamidato-*N*)cobalt(*III*)(2+), 10Cl

Pentammine(2-carboxamidobenzonitrile)cobalt(III)(2+)

[68893-64-1]



M 289.2 (ion)

NCC_6H_4CONH ligand, formed from Pentaammine(1,2-dicyanobenzene)cobalt(*III*)(3+), IC-006160.

Perchlorate: [69120-37-2].
Orange solid. Sol. DMSO.
▷ Potentially explosive.

Balahura, R.J., *Inorg. Chem.*, 1979, **18**, 937 (*synth, ir, pmr, uv*)

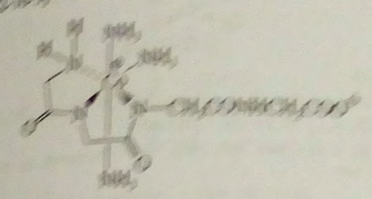
IC-006206

$C_6H_{24}CoN_8O_8$

Triammine[tetraglycinato(3−)]cobaltate(*III*)

*Triammine[bis(μ-[bis(2-glycinato)-*O,N,O'*]glycinato-*O,O'*)]cobaltate(3−)*

[83252-16-5]



M 359.2

Prob. sonlig. shown. Orange solid + $2H_2O$. Converts to Triammine[tetraglycinato(3−)]cobalt(*III*)(2+), IC-006209 at pH 1.

Hawkins, C.J. *et al. Inorg. Chem.*, 1982, **21**, 3681 (*synth, prev. str, pmr*)

$C_8H_{20}CoO_2P_2S_4$ IC-006207

Bis(*O,O*-diethylphosphorodithioato-*S,S'*)cobalt(*II*), 9Cl

Bis(diethyldithiophosphato)cobalt(II)

Bis(diethoxydithiophosphinato)cobalt(II)

[38625-31-9]

M 429.3

Probably tetrahedral. Lustrous flat blue needles. Sol. hot CH_2Cl_2. Paramagnetic.

Cavell, R.G., *Inorg. Chem.*, 1972, **11**, 1759 (*synth., ir, magnetism, uv*)

$C_8H_{20}CoS_4^{2\ominus}$ IC-006208

Tetrakis(ethanethiolato)cobaltate(*II*)(2−), 11Cl

Tetrakis(ethylthio)cobaltate(II)(2−)

Tetrakis(ethylmercapto)cobaltate(II)(2−)

$[Co(SEt)_4]^{2\ominus}$

M 303.4 (ion)

Probably tetrahedral.

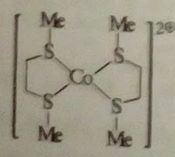
Bis-Me_4N salt: [88271-65-2].
Deep blue needles. Sol. $CHCl_3$, MeCN.

Hagen, K.S. *et al. Inorg. Chem.*, 1984, **23**, 418 (*synth, str., pmr*)

$C_8H_{20}CoS_4^{2\oplus}$ IC-006209

Bis(2,5-dithiahexane)cobalt(*II*)(2+)

*Bis[1,2-bis(methylthio)ethane-*S,S'*]cobalt(2+)*



M 303.4 (ion)

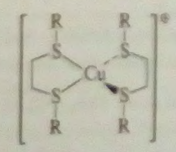
Diperchlorate: [14873-90-6].
$C_8H_{20}Cl_2CoO_8S_4$ M 502.3
Pink cryst. Insol. common org. solvs. V. spar. sol. $MeNO_2$. Paramagnetic. Example of two ClO_4 ligands both co-ordinating in solid state.

Bailey, N.A. *et al. J. Chem. Soc. A*, 1968, 1592 (*synth, ir, magnetism*)
Nakano, M. *et al. Bull. Chem. Soc. Jpn.*, 1979, **52**, 2563 (*synth, ir, uv-vis, cis and trans-forms, resolv*)
Matsumoto, K. *et al. Bull. Chem. Soc. Jpn.*, 1982, **55**, 1840 (*cryst struct, cis-form, abs config*)
Blasius, E. *et al. Z. Anorg. Allg. Chem.*, 1984, **509**, 167 (*synth, uv-vis, ir*)

$C_8H_{20}CuS_4^{\oplus}$ IC-006211

Bis(2,5-dithiahexane)copper(*I*)(1+)

Bis[1,2-bis(methylthio)ethane-S,S']copper(1+), 10Cl



R = Me

M 308.0 (ion)

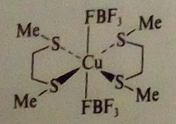
Distorted tetrahedral geometry. See also Hexakis[μ-[1,2-bis(methylthio)ethane-*S*:*S*']]tricopper(4+), *IC-011667*.
Twinned crystals.
Tetrafluoroborate: [62207-31-2].
White cryst. (MeOH). Mp 155-156°.
Perchlorate: [62207-32-3].
White cryst. (MeOH).
▷ Potentially explosive.

Ainscough, E.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2375 (*synth, ir, vis*)

IC-006212

$C_8H_{20}CuS_4^{2\oplus}$

Bis(2,5-dithiahexane)copper(*II*)(2+)
Bis[1,2-bis(methylthio)ethane-S:S']copper(2+), 10CI



tetrafluoroborate salt

M 308.0 (ion)
Distorted octahedral struct.
Bis-tetrafluoroborate: [71120-66-6].
Deep-red cryst. (EtOH).
Diperchlorate: [21444-14-4].
Mp 160° explodes.
▷ Explodes violently when dry or on heating; risk of explosion during Flint's synthesis.

Flint, C.D. *et al*, *J. Chem. Soc. A*, 1968, 2178 (*synth, haz*)
Ainscough, E.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2375 (*synth, ir*)
Baker, E.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 877 (*synth, cryst struct*)
Sakaguchi, U. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 600 (*esr*)

IC-006213

$C_8H_{20}F_4N_2W$

Bis(diethylamido)tetrafluorotungsten(*VI*)

$WF_4(NEt_2)_2$

M 404.1
Polymeric via F bridges. Synth. from WF_6 and $2Me_3SiNEt_2$ at 20° for 12h. Similar in physical and chemical props to WF_5NEt_2. Dark red, viscous liq. d_4^{20} 1.972.

Majid, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1876 (*synth, pmr, ir*)

IC-006214

$C_8H_{20}FeO_4^{\ominus}$

Tetraethoxyferrate(*III*)(1–)

$[Fe(OEt)_4]^{\ominus}$

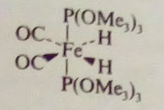
M 236.0 (ion)
Component of $EtOH/EtO^{\ominus}/Fe(III)$ system. $[Fe(OEt)_6]^{3\ominus}$ also present.
Na salt: [61420-80-2].
Synth. from $NaOEt + Fe(OEt)_3 + EtOH$.

Jain, N.C. *et al*, *Proc. - Indian Acad. Sci., Sect. A*, 1976, **84**, 98 (*detection*)
Chernova, N.A. *et al*, *Koord. Khim.*, 1985, **11**, 1240 (*synth*)

IC-006215

$C_8H_{20}FeO_8P_2$

Dicarbonyldihydrobis(trimethyl phosphite-*P*)iron, 11CI
[77482-07-6]



M 362.0
Colourless needles (pet. ether). Mp 29°. Ir ν_{CO} 2012s, 1972s; ν_{FeH} 1920s cm^{-1} (hexane).

Berke, H. *et al*, *Chem. Ber.*, 1981, **114**, 2754 (*synth, ir, pmr, P-31 nmr, ms*)

IC-006216

$C_8H_{20}GaS_4^{\ominus}$

Tetrakis(ethanethiolato)gallate(*III*)(1–)
Tetrakis(ethylmercapto)gallate(III)(*1–*)

$[Ga(SEt)_4]^{\ominus}$ (T_d)

M 314.2 (ion)
Tetrapropylammonium salt: [101165-29-1].
Synth. from $GaCl_3$, LiSEt, and $[Pr_4N]Br$ in EtOH.
White air stable solid (DMF/Et_2O).

Maelia, L.E. *et al*, *Inorg. Chem.*, 1986, **25**, 1896 (*synth, cryst struct*)

IC-006217

$C_8H_{20}GeO_4$

Germanium(*IV*) ethoxide
Tetraethoxygermane. Germanium tetraethoxide
[19639-26-0]

$Ge(OEt)_4$

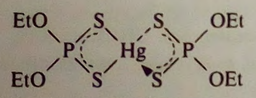
M 252.8
Colourless liq. Mp –81°. Bp 185.5°.

Skobeleva, S.E. *et al*, *Dokl. Akad. Nauk SSSR*, 1973, **210**, 122 (*ir*)
Shreider, V.A. *et al*, *Inorg. Chim. Acta*, 1981, **53**, L73 (*synth*)
Grinberg, E.E. *et al*, *Khim. Promst.* (*Moscow*), 1986, **5**, 263 (*synth*)

IC-006218

$C_8H_{20}HgO_4P_2S_4$

Bis(*O,O*-diethyl phosphorodithioato-*S,S'*)mercury, 9CI
Bis(dihydrogen phosphorodithioato)mercury-O,O,O',O'-tetraethyl ester, 8CI. Ethyl mercury phosphorodithioate
[19582-90-2]



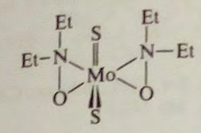
M 571.0
White cryst. (C_6H_6). Insol. MeCN. Mp 124° ; 129°.
[1446-05-5]

Hu, P.-F. *et al*, *CA*, 1958, **52**, 7186 (*synth*)
Toropova, V.F. *et al*, *J. Gen. Chem. USSR* (*Engl. Transl.*), 1967, **37**, 679 (*stability const*)
Adams, D.M. *et al*, *J. Chem. Soc. A*, 1968, 1299 (*ir*)
Cheremisina, I.M. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1971, 2150 (*ir*)
Geloso, C. *et al*, *Can. J. Chem.*, 1987, **65**, 928 (*synth, P-31 nmr, ir, pmr*)

IC-006219

$C_8H_{20}MoN_2O_2S_2$

Bis(*N,N*-diethylhydroxylaminato-*N,O*) disulfidomolybdenum(*VI*)
Bis(N-ethyl-N-hydroxyethanaminato-N,O) dithioxomolybdenum(VI), *10CI*
[76900-53-3]



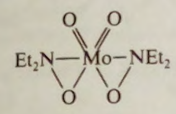
M 336.3
Pseudo-tetrahedral geometry. Violet-red cryst.
[84472-65-1]

Hofer, E. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1981, **20**, 282 (*synth*)
Gheller, S.F. *et al*, *Aust. J. Chem.*, 1982, **35**, 2183 (*cryst struct*)
Wieghardt, V.K. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **492**, 164 (*synth, ir*)
Minelli, M. *et al*, *Inorg. Chem.*, 1983, **22**, 3952 (*Mo-95 nmr*)

IC-006220

$C_8H_{20}MoN_2O_4$

Bis(*N,N*-diethylhydroxylaminato)dioxomolybdenum(*VI*)
Bis(N-ethyl-N-hydroxyethanaminato-N,O) dioxomolybdenum(VI), *11CI, 10CI*
[74081-86-0]



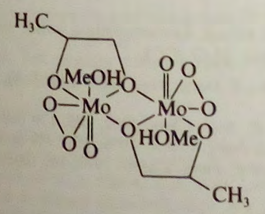
M 304.1
Synth. from $HONEt_2$ + MoO_3 or $Na_2MoO_4.2H_2O$.
Colourless cryst. (H_2O). Sol. $CHCl_3$, DMSO; spar. sol. H_2O. Mp 137°. Ir ν_{MoO} 905 cm^{-1} (KBr).

Saussine, L. *et al*, *Nouv. J. Chim.*, 1980, **4**, 235 (*cryst struct, synth, reactions*)
Minelli, M. *et al*, *Inorg. Chem.*, 1983, **22**, 3952 (*Mo-95 nmr*)
Wieghardt, K. *et al*, *Inorg. Chem.*, 1980, **19**, 2927; 1981, **20**, 3436 (*synth, ir, pmr, reactions*)

IC-006221

$C_8H_{20}Mo_2O_{12}$

Bis(methanol)dioxodiperoxybis[μ-[1,2-propanediolato(2–)-O^1:O^1,O^2]]dimolybdenum(*VI*), 11CI
Bis[(μ_2-propane-1,2-diolato-O,O,O')oxoperoxomethanolmolybdenum(VI)]
[104946-40-9]



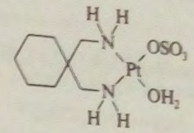
M 500.1
Planar Mo_2O_2 core; interatomic distance Mo—Mo 339.5 pm. The peroxy and diolate oxygens form the equatorial plane of a distorted pentagonal bipyramid. First structurally characterised non-ionic polynuclear Mo(*VI*) peroxo complex with covalently-bonded diolate ligand. Moisture-sensitive bright yellow cryst. + 2MeOH. Dec. to molybdenum blue at r.t.

Shum, W., *Inorg. Chem.*, 1986, **25**, 4329 (*cryst struct*)

IC-006222

$C_8H_{20}N_2O_5PtS$

Aqua[1,1-bis(aminomethyl)cyclohexane] sulfatoplatinum(*II*)
Aqua[1,1-cyclohexanedimethanamine][sulfato(2–)-O]platinum(II), *11CI*
[80669-94-9]



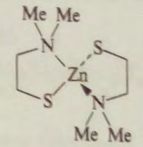
M 451.4
Square planar struct. with monodentate $SO_4^{2\ominus}$. Synth. from $Pt[C_6H_{10}(CH_2NH_2)_2]Cl_2$ + Ag_2SO_4. Antineoplastic agent. Cryst.; forms a monohydrate.
[104005-21-2]

Rose, W.C. *et al*, *Cancer Treat. Rep.*, 1982, **66**, 135 (*props*)
Meinema, H. *et al*, *Inorg. Chim. Acta*, 1986, **114**, 127 (*synth, cryst struct*)

IC-006223

$C_8H_{20}N_2S_2Zn$

Bis[2-(dimethylamino)ethanethiolato-*N,S*]zinc, 9CI
Zinc 2-(dimethylamino)ethanethiolate
[41755-11-7]



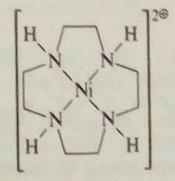
M 273.7
Tetrahedral Zn; monomeric in soln. Cryst. (MeOH); dec. in H_2O and in acid and base. Sol. MeOH, EtOH, Me_2CO, Et_2O, MeCN, CH_2Cl_2; sl. sol. hexane.

Mittal, M.L. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1691 (*stability const*)
Casals, I. *et al*, *Polyhedron*, 1990, **9**, 763 (*synth, cryst struct*)

IC-006224

$C_8H_{20}N_4Ni^{2\oplus}$

(1,4,7,10-Tetraazacyclododecane)nickel(*II*)(2+), 9CI
(Cyclen)nickel(2+). ([12]AneN$_4$)nickel(2+)
[56647-83-7]



M 230.9 (ion)
Smallest macrocycle to give square planar Ni(*II*). Exists in equilibrium with bis-aqua complex in H_2O. Counteranions tend to coordinate to metal centre.
Dichloride: [58117-52-5]. *Dichloro(1,4,7,10-tetraazacyclododecane)nickel*(II)
$C_8H_{20}Cl_2N_4Ni$ M 301.8
Purple solid. Octahedral compd. Paramagnetic.
Diperchlorate: [71911-56-3].
$C_8H_{20}Cl_2N_4NiO_8$ M 429.8
Yellow in soln. Not isol. Perchlorate moieties may coordinate to nickel.

▷ Potentially explosive.

[63598-05-0]

Smierciak, R. *et al, Inorg. Chem.*, 1977, **16**, 2646 (*synth, uv, magnetism*)
Fabbrizzi, L. *et al, Inorg. Chem.*, 1977, **16**, 2667 (*uv*)
Plassman, W.H. *et al, Inorg. Chem.*, 1980, **19**, 1101 (*uv, magnetism*)
Coates, J.H. *et al, Inorg. Chem.*, 1981, **20**, 707 (*O-17 nmr*)

IC-006225

$C_8H_{20}N_4NiS_4^{2\oplus}$

Tetrakis(thioacetamide)nickel(*II*)(2+), 8CI

Tetrakis(ethanethioamide-S)*nickel*(II)(2+), *9CI*

$$Ni[S{=}C(NH_2)CH_3]_4^{2\oplus}$$

M 359.2 (ion)

Square planar. Ligand coordinates through S atom.

Dibromide: [19615-62-4].
$C_8H_{20}Br_2N_4NiS_4$ M 519.0
Blue-purple solid or red cryst.

Flint, C.D. *et al, J. Chem. Soc. A*, 1968, 750 (*synth, ir, uv*)
Spofford, W.A. *et al, Inorg. Chim. Acta*, 1971, **5**, 70 (*synth, cryst struct*)

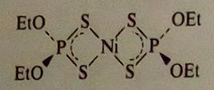
IC-006226

$C_8H_{20}NiO_4P_2S_4$

Bis(*O,O'*-diethyldithiophosphato)nickel(*II*)

Bis(dihydrogenphosphorodithioato) tetraethylester nickel, 8CI. Bis(diethylphosphorodithioato-S,S')*nickel, 9CI*

[16743-23-0]



M 429.1

Square planar struct. Forms many complexes with neutral ligands. Deep purple cryst. Sol. H_2O, many org. solvs.

Joørgensen, C.K., *J. Inorg. Nucl. Chem.*, 1962, **24**, 1572 (*synth, uv*)
McConnell, J.F. *et al, Acta Crystallogr., Sect. B*, 1967, **22**, 853 (*cryst struct*)
Rudzinski, W. *et al, Inorg. Chem.*, 1977, **16**, 1206 (*ir*)
Szczepaniak, W. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1981, **55**, 2289 (*ms*)

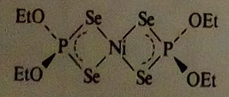
IC-006227

$C_8H_{20}NiO_4P_2Se_4$

Bis(diethyldiselenophosphato)nickel(*II*)

Bis(O,O-*diethylphosphorodiselenoato*-Se,Se')*nickel, 9CI. Bis(dihydrogen phosphorodiselenato)nickel*, O,O,O,O-*tetraethylester, 8CI*

[55516-90-0]



M 616.7

Square planar coordn. around Ni; tetrahedral coordn. around P. Synth. from $Ni(ClO_4)_2$ + $(EtO)_2PSe_2K$. Monoclinic, grey cryst. (EtOH). Mp 102°. Diamagnetic.

[33774-62-8]

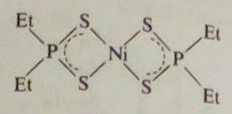
Krishnan, V. *et al, J. Coord. Chem.*, 1971, **1**, 1 (*synth, ir, uv*)
van der Leemput, P.J.H.A.M. *et al, Cryst. Struct. Commun.*, 1975, **4**, 167 (*cryst struct*)

$C_8H_{20}NiP_2S_4$

Bis(diethylphosphinodithioato-*S,S'*)nickel, 9CI IC-006228

Bis(diethylphosphorodithioato)nickel(II)

[15392-73-1]



M 365.1

Blue-purple tablets. Sol. C_6H_6, toluene, $CHCl_3$; insol. dioxan, alcohols. Mp 142.5°.

[15701-66-3]

Kuchen, W. *et al, Chem. Ber.*, 1965, **98**, 3981 (*synth*)
Shetty, P.S. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 1294 (*cryst struct*)
Nanjo, M. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 2411 (*ir, pmr*)
Heinz, S. *et al, Org. Mass Spectrom.*, 1984, **19**, 82 (*ms*)

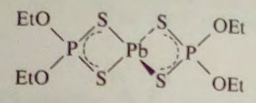
IC-006229

$C_8H_{20}O_4P_2PbS_4$

Bis(*O,O*-diethyl phosphorodithioato-*S,S'*)lead

Lead(II) *diethyldithiophosphate. Phosphorodithioic acid,* O,O-*diethyl ester, lead(2+) salt, 9CI*

[1068-23-1]



M 577.6

Synth. from $(EtO)_2P(S)SK$ + $Pb(OAc)_2$. Prismatic needles (Et_2O). Mp 75-76°.

[16569-73-6]

Szczepaniak, W. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1982, **56**, 469 (*ms*)
Ito, T., *Acta Crystallogr., Sect. B*, 1972, **28**, 1034 (*cryst struct*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1968, 1299 (*ir*)
Mastin, T.W. *et al, J. Am. Chem. Soc.*, 1945, **67**, 1662 (*synth*)

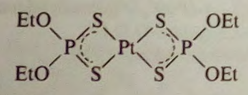
IC-006230

$C_8H_{20}O_4P_2PtS_4$

Bis(diethyldithiophosphato)platinum(*II*)

Bis(O,O-*Diethylphosphorodithioato)platinum, 10CI. Ethylplatinumphosphorodithioate*

[37583-01-0]



M 565.5

Square planar struct. Lemon-yellow solid, can be solv.-extracted. Sol. H_2O, CCl_4.

Joergensen, C.K., *J. Inorg. Nucl. Chem.*, 1962, **24**, 157 (*synth, uv-vis*)
Bode, H. *et al, Z. Anal. Chem*, 1962, **185**, 179 (*solv extraction*)
Maier, J.P. *et al, Inorg. Chem.*, 1976, **15**, 1989 (*pe*)
Rudzinski, W. *et al, Inorg. Chem.*, 1977, **16**, 1206 (*ir*)

IC-006231

$C_8H_{20}O_4P_2S_4Zn$

Bis(*O,O*-diethylphosphorodithioato-*S,S'*)zinc

Zinc diethyldithiophosphate. Ethyl zinc phosphorodithioate

[7268-60-2]

$$[(EtO)_2PSS]_2Zn$$

M 435.8

In the struct., one dithiophosphate group is coordinated to a single Zn atom by its 2 S atoms, while the other bridges 2 different Zn atoms forming infinite, linear zig-zag chains. Prepd. from P_2S_5 + EtOH + $Zn(OAc)_2$. Cryst. Mp 77°.

[16569-75-8]

Ito, T. *et al, Acta Crystallogr., Sect. B*, 1969, **25**, 2303 (*cryst struct*)
Dakternieks, D.R. *et al, Aust. J. Chem.*, 1970, **23**, 1989 (*synth, ir*)
Szczepaniak, W. *et al, Pol. J. Chem.* (*Rocz. Chem.*), 1981, **55**, 2289 (*ms*)

IC-006232

$C_8H_{20}O_4Sn$

Tin(*IV*) ethoxide

Ethanol, tin(4+) salt, 9CI. Ethyl stannate. Tetraethoxytin. Tetraethoxystannane

[3173-69-1]

$$Sn(OEt)_4$$

M 298.9

Prepd. from $SnCl_4$ + NaOEt. White solid.

Bradley, D.C. *et al, J. Chem. Soc.*, 1957, 4775 (*synth*)
Maire, J.C., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1960, **251**, 1292 (*synth*)
Multani, R.K., *Indian J. Chem.*, 1964, **2**, 335 (*synth*)

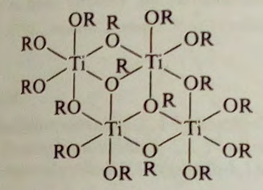
IC-006233

$C_8H_{20}O_4Ti$

Titanium(*IV*) ethoxide

Tetraethoxytitanium(IV). *Titanium tetraethoxide*

[3087-36-3]



tetramer

R = Et

M 228.1

Monomer unknown. Usually tetrameric, but may be trimeric in soln. (Martin, 1961). Synth. from $TiCl_4$ + NaOEt or from $TiCl_4$ + EtOH + NH_3 in C_6H_6 and purif. by dist. Commercially available. Can be used in olefin polymerisation catalysts and in formation of TiO_2 thin film capacitors. Bp_5 133°, $Bp_{0.1}$ 103°.

▷ Flammable.

Tetramer: Hexadecaethoxytetratitanium(IV)
$C_{32}H_{80}O_{16}Ti_4$ M 912.4
White solid, but usually colourless oily liq. at r.t. Readily hydrol. Sol. C_6H_6.

[3087-36-3]

Crowe, R.W. *et al, J. Am. Chem. Soc.*, 1950, **72**, 1694 (*synth*)
Bradley, D.C. *et al, J. Chem. Soc.*, 1952, 2773 (*synth*)
Barraclough, C.G. *et al, J. Chem. Soc.*, 1961, 2601 (*ir*)
Bradley, D.C. *et al, Nature* (*London*), 1961, **191**, 273 (*struct*)
Martin, R.L. *et al, Nature* (*London*), 1961, **191**, 274 (*struct*)
Ibers, J.A., *Nature* (*London*), 1963, **197**, 686 (*cryst struct, tetramer*)
Sakurai, S. *et al, Rev. Electr. Commun. Lab.*, Tokyo, 1963, **11**, 178; *CA*, **59**, 8232a (*use*)
Hoever, H. *et al, Ann. Chem.*, 1965, **685**, 89 (*use*)

$C_8H_{20}O_4U$

Tetraethoxyuranium(*IV*) IC-006234

Uranium(IV) *ethoxide. Uranium tetraethoxide*

[64653-70-9]

$$U(OEt)_4$$

M 418.2

V. air- and water-sensitive light-green solid. Sl. sol. EtOH.

Jones, R.G. *et al, J. Am. Chem. Soc.*, 1956, **78**, 4285 (*synth*)
Vilenha, M.T. *et al, Inorg. Chim. Acta*, 1984, **95**, 11 (*synth*)

$C_8H_{20}O_6P_2$

Tetraethyl hypophosphate, 9CI IC-006235

Tetraethoxydiphosphine dioxide. Tetraethoxodiphosphane

[679-37-8]

$$(EtO)_2P(O){-}P(O)(OEt)_2$$

M 274.1

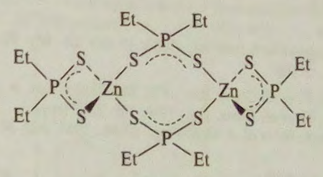
Liq. d_4^{20} 1.17. $Bp_{0.01}$ 88-89°. n_D^{20} 1.4394.

Baudler, M., *Z. Anorg. Allg. Chem.*, 1956, **288**, 171 (*synth, props, raman*)
Michalski, J. *et al, Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1965, **13**, 253 (*synth*)
Harris, R.K. *et al, J. Chem. Soc. A*, 1967, 37 (*pmr, P-31 nmr*)
Mowthorpe, D.J. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 451 (*P-31 nmr, pmr*)
Stec, W.J. *et al, Org. Mass Spectrom.*, 1975, **10**, 485 (*ms*)

$C_8H_{20}P_2S_4Zn$

Bis(diethylphosphinodithioato-*S,S'*)zinc(*II*) IC-006236

[15227-14-2]



dimer

M 371.8

Dimeric in solid state, partial dissoc. in C_6H_6.

Dimer: [28771-10-0]. *Bis*[*μ*-(*diethylphosphinodithioato*-S:S')] *bis(diethylphosphinodithioato*-S,S')*dizinc, 11CI*
$C_{16}H_{40}P_4S_8Zn_2$ M 743.6
Colourless prisms (EtOH/C_6H_6). Sol. $CHCl_3$. Mp 166.5-167°.

[21380-00-7]

Kuchen, W. *et al, Chem. Ber.*, 1964, **97**, 2306; 1968, **101**, 1991 (*synth*)
Calligaris, M. *et al, J. Chem. Soc. A*, 1970, 714 (*cryst struct*)
McCleverty, J.A. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 627 (*synth, P-31 nmr*)

IC-006237

$C_8H_{20}S_4U$

Tetrakis(ethanethiolato)uranium(*IV*)

Uranium(IV) *ethylmercaptide. Tetrakis(ethylmercapto) uranium*(IV)

$$U(SEt)_4$$

M 482.5

V. air- and moisture-sensitive green solid.

▷ Pyrophoric in air.

Jones, R.G. *et al, J. Am. Chem. Soc.*, 1956, **78**, 4285 (*synth*)

IC-006238

$C_{12}H_{32}B_2Cl_2Co_2Si_4$

6-Cl-(chlorogermyl)-2,3-bis(trimethylsilyl)-2,3-dicarba-1-germahexaborane(6), 1ICl

2,3-Bis(trimethylsilyl)-5-(μ-chlorogermyl)-2,3-dicarba-1-germahexaborane(6)

[81967-92-0]

M 468.2

Green. Air- and moisture-sensitive colourless cryst. ($CHCl_3$). Sol. THF, CCl_4, $CHCl_3$, CH_2Cl_2, C_6H_6, hexane. Mp 67°

Siewerthin, U. et al. Organometallics, 1998, 5, 1890 (synth, cryst struct, ir, pmr, cmr, B-11 nmr, Si-29 nmr, ms)

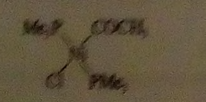
IC-006239

$C_{14}H_{31}ClNOP_2$

Acetylchlorobis(trimethylphosphine)nickel(II), 9Cl

Chloroacetylchlorobis(trimethylphosphine)nickel(II)

[65081-75-3]



M 289.3

***trans*-form**

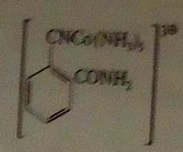
Orange-yellow needles, stable to dry air. Mp 98-99°. Dec. > 108°

Klein, H.F. et al. Chem. Ber., 1976, 109, 2524 (synth, ir, pmr)
Hübner, G. et al. Chem. Ber., 1976, 109, 2533 (struct)
Bochmann, M. et al. J. Organomet. Chem., 1987, 332, 141 (props)

IC-006240

$C_{14}H_{21}CoN_7O^{2\oplus}$

Pentaammine(2-cyanobenzamide-N^1)cobalt(III)(3+), 3ICl



M 290.2 (ion)

Triperchlorate: [69120-41-8].
No phys. props. reported.

Balaitura, R.J. et al. Inorg. Chem., 1979, 18, 937; 1981, 20, 4159 (synth, ir, pmr, kinetics)

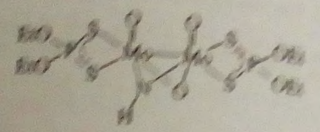
IC-006241

$C_4H_{22}Mo_2NO_2P_2S_4$

Bis(O,O-diethylphosphorodithioato-S,S')-μ-imido-μ-oxodioxodimolybdenum(VI), 10Cl

μ-Imido-μ-oxobis(O,O-diethyldithiophosphato)molybdenum(VI)

[66161-06-2]



M 625.3

Fawnbery yellow cryst. (C_6H_6/heptane).

Edelblut, A.W. et al. J. Am. Chem. Soc., 1972, 100, 2256 (cryst struct)
Edelblut, A.W. et al. Inorg. Chem., 1980, 19, 2066 (synth)

IC-006242

$C_8H_{22}AlN_2O_3^{\ominus}$

Bis(2-(dimethylamino)ethanolato-N,O) dihydroaluminate(1−)

$[AlH_2(OCH_2CH_2NMe_2)_2]^{\ominus}$

M 205.2 (ion)
Several related species descr.

Na salt: [22356-32-5].
Synth. from $NaAlH_4$ and $NaAl(OCH_2CH_2NMe_2)_2$. Selective reducing agent e.g. for esters to aldehydes and as catalyst for formation Grignard reagents. Viscous colourless moisture-sensitive liq. Usually used *in situ*

Machácek, J. et al. Collect. Czech. Chem. Commun., 1973, 38, xx (synth, props)

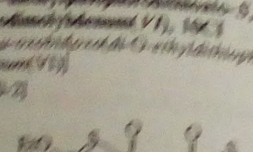
IC-006243

$C_8H_{22}B_2N_6$

2,2'-Hydrazobis[1,3-dimethyl-1,3,2-diazaborolidine], 10Cl

N,N'-Bis-2-(1,3-dimethyl-1,3,2-diazaboracyclopentyl) hydrazine. N,N'-Bis(1,3-dimethyl-1,3,2-diazaborolan-2-yl) hydrazine

[62367-27-5]



M 223.9
Moisture-sensitive low-melting solid; fairly stable under reduced pressure and can be distilled. Mp 36-41°. $Bp_{0.1}$ 80-83°.

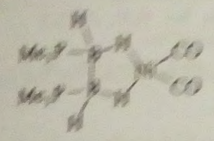
Christmas, B.K. et al, Z. Naturforsch., B, 1977, 32, 157 (synth, ir, nmr, ms)
Niedenzu, K. et al, Z. Anorg. Allg. Chem., 1978, 439, 103 (nmr, props)
Bharara, P.C. et al, Z. Naturforsch., B, 1979, 34, 1352

IC-006244

$C_5H_{18}NO_2P_2$

Bis(dimethylphosphito)(trimethylphosphine)dihydrotriborate(1−), 11Cl

[68606-86-9]



M 201.9
H-B(H)-H units readily broken by donors. Green-yellow solid (toluene/pentane), mod. stable in air, but dec. in CH_2Cl_2 soln.

Imoto, H. et al, Inorg. Chem., 1985, 24, 709; 1987, 26, 1397 (synth, pmr, B-11 nmr, ir, ms, xray)

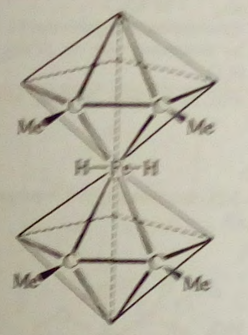
IC-006245

$C_{10}H_{22}B_2Fe$

Bis[(2,3,4,6-η)-pentahydro-4,5-dimethyl-4,5-dicarbahexaborato(1−)-H^6]iron, 9Cl

Bis(2,3-dimethyl-2,3-dicarbahexaborane dihydride. [2,3-$(C_2B_4H_4(CH_3)_2)_2Fe^{II}H_2$

[58046-86-9]



M 260.5
H-Fe-H atoms not located. Extremely air-sensitive deep-red cryst. Subl. 0° *in vacuo*.

Maxwell, W.M. et al, Inorg. Chem., 1976, 15, 1343 (synth, nmr, pmr, ms, ir)
Pipal, J.R. et al, Inorg. Chem., 1979, 18, 263 (synth, struct)

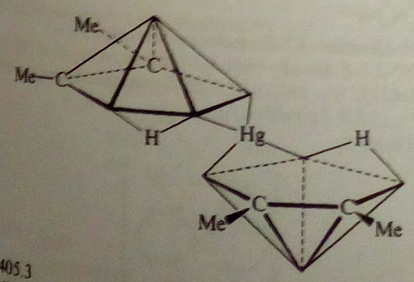
IC-006246

$C_8H_{22}B_2Hg$

Bis[(4,5-η)-pentahydro-2,3-dimethyl-2,3-dicarbahexaborato(1−)]mercury, 10Cl

Bis(2,3-dimethyl-2,3-dicarbahexaboran(8)-4-yl)mercury, 10Cl

[73608-23-8]



M 405.3
Sublimable cryst. Survives brief exposure to air.

[59879-61-7]

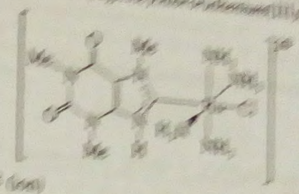
Bowman, W.R. et al, Inorg. Chem., 1979, 18, 1999 (synth, ir, pmr, cmr, ms, B-11 nmr)

IC-006247

$C_{36}H_{42}ClN_{12}O_2Ru^{\oplus}$

Tetrammine(1H-2,3,4,6,7,8-hexahydro-1,3,7,9-tetramethyl-2,6-dioxo-4H-purin-4-ylidene)ruthenium(2+), 3Cl

Tetrammine(1,3,7,9-tetramethyluricine)ruthenium(III) (2+). Tetrammine(caffeine)chlororuthenium(III)(2+)



M 598.8 (ion)
trans-Octahedral

Bichloride: [55208-42-9].
Synth. from Pentammine(aqua)ruthenium(II)(2+), IC-(109569) + caffeine, followed by aerial oxidation and ion-exchange chromatog. Red cryst. (1.*M* HCl, EtOH). λ_{max} 350 (109).

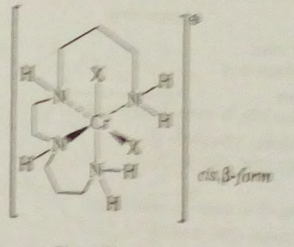
Clarke, M.J. et al, J. Am. Chem. Soc., 1975, 97, 3307 (synth, ir, pKa, electrochem)

IC-006248

$C_{20}H_{52}Cl_3CrN_8^{\oplus}$

Dichloro(1,10-diamino-4,7-diazadecane)chromium(III) (1+)

Dichloro[N,N'-(1,2-ethanediyl)bis(1,3-propanediamine)-N,N',N'',N'']chromium(1+), 1ICl, 1HCl, 3Cl



cis-β-form

X = Cl

M 297.1 (ion)
Octahedral cation.

cis*-β-*form
Has been resolved. Analogues with X = H_2O, $OH^{\ominus}$ etc. also known.

Perchlorate: Violet cryst.

***trans*-form**
Has been resolved. Synth. from $CrCl_3$ in DMF + Zn powder + ligand. Analogues with X = $NCS^{\ominus}$, $OH^{\ominus}$, H_2O with trans-octahedral struct. also known.

Chloride: Green cryst. (2.*M* HCl at 80°).
Nitrate: [81688-78-0].
Green cryst.
Perchlorate: Green cryst. (2.*M* HCl at 100°). Sl. sol. H_2O.

[53567-41-2, 53625-78-8, 53625-80-2, 74679-98-4, 81738-84-3, 81739-51-7]

Bosnich, B. et al, Inorg. Chem., 1975, 14, 815, 828 (synth, cd)
Yang, D. et al, Inorg. Chem., 1982, 21, 2999 (synth, uv, resol, cd, reactions)
House, D.A. et al, Inorg. Chim. Acta, 1983, 70, 13 (kinetics)

IC-006249

$C_8H_{22}Cl_2FeN_2$

Bis(butylamine)dichloroiron(*II*)

Iron(II) *chloride bis(butylamine)*

$FeCl_2(NH_2CH_2CH_2CH_2CH_3)_2$

M 273.0

Synth. from $FeCl_2$ or $FeCl_3$ + butylamine. White solid. $\mu_{eff} = 5.5\mu_B$.

McGregor, W.R. *et al, J. Inorg. Nucl. Chem.*, 1966, **28**, 1027 (*synth, ir, magnetism*)

IC-006250

$C_8H_{22}Cl_2P_2Pd$

Dichlorobis(diethylphosphine)palladium(*II*)

$PdCl_2(PHEt_2)_2$

M 357.5

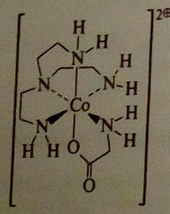
Synth. from Na_2PdCl_4 + Et_2PH. White needles (Me_2CO). Mp 170°.

Hayter, R.G. *et al, Inorg. Chem.*, 1963, **2**, 306 (*synth*)

IC-006251

$C_8H_{22}CoN_5O_2^{2\oplus}$

Glycinato[tris(2-aminoethyl)amine]cobalt(*III*)(2+)



orange-form

M 279.2 (ion)

Two isomers exist.

Orange-form

Glycine-NH_2 is *trans*- to *tert*-amine.

Diperchlorate: [29414-69-5].

Orange cryst. (aq. $HClO_4$).

Red-form

Glycine-O is *trans*- to *tert*-amine.

Diperchlorate: [29414-64-0].

Red needles (H_2O).

[56978-05-3, 81623-45-2, 81623-46-3]

Mitsui, Y. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 2095 (*cryst struct*)

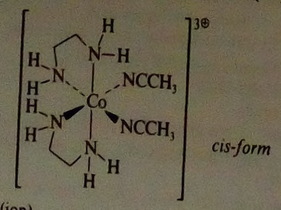
Jackson, W.G. *et al, J. Am. Chem. Soc.*, 1981, **103**, 533 (*synth*)

Wautier, H. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 2479 (*synth*)

$C_8H_{22}CoN_6^{3\oplus}$

IC-006252

Bis(acetonitrile)bis(ethylenediamine)cobalt(*III*)(3+)



cis-form

M 261.2 (ion)

Octahedral.

cis-form

Nitrate, diperchlorate: [75522-65-5].

Orange-yellow needles. Sol. H_2O, DMSO.

▷ Potentially explosive.

trans-form

Triperchlorate: [75557-19-6].

Yellow needles. Sol. H_2O, DMSO.

▷ Potentially explosive.

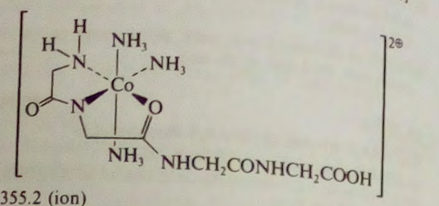
Dixon, N.E. *et al, Inorg. Chem.*, 1981, **20**, 470 (*synth, ur, pmr*)

$C_8H_{22}CoN_7O_5^{2\oplus}$

IC-006253

Triammine[tetraglycinato(1−)]cobalt(*III*)(2+)

Triammine[N-[N-(N-*glycylglycyl*)*glycyl*]*glycinato*(2−)]*cobalt*(1+), *11Cl*



M 355.2 (ion)

Dinitrate: [82536-80-9].

$C_8H_{22}CoN_9O_{11}$ M 479.2

Obt. from Triammine[tetraglycinato(3−)]cobalt(*III*), IC-006206 by treatment with dil. HNO_3 at pH 1. Pink solid. Sol. H_2O.

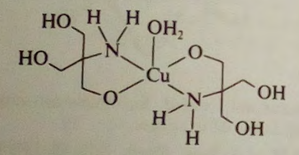
Hawkins, C.J. *et al, Inorg. Chem.*, 1982, **21**, 3681 (*synth, pmr, cmr, uv-vis*)

$C_8H_{22}CuN_2O_7$

IC-006254

Bis[2-amino-2-(hydroxymethyl)-1,3-propanediolato-*N,O*]aquacopper(*II*)

[111835-03-1]



M 321.8

Blue cryst. + $5H_2O$ (aq. sol... at pH 10). Sol. H_2O.

Austrilino, L. *et al, Can. J. Chem.*, 1987, **65**, 821 (*synth, cryst struct, esr*)

Mazus, M.D. *et al, Zh. Neorg. Khim.* 1987, **32**, 2212 (*synth, cryst struct*)

Polyakov, V.N. *et al, Zh. Neorg. Khim.*, 1989, **34**, 1500 (*synth, ir, esr, magnetism*)

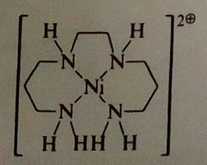
$C_8H_{22}N_4Ni^{2\oplus}$

IC-006255

(1,10-Diamino-4,7-diazadecane)nickel(*II*)(2+)

[N,N″-*1,2-Ethanediylbis*[*1,3-propanediamine*]-N,N′,N″,N‴]*nickel*(II)(2+), *10Cl*. (*1,5,8,12-Tetraazadodecane*)*nickel*(II)(2+). (*3,2,3-Tet*)*nickel*(2+)

[63528-06-3]



M 232.9 (ion)

Iodide forms as square planar (yellow) and octahedral (lilac) forms. Other salts and solns. octahedral.

Diiodide: [68894-66-6].

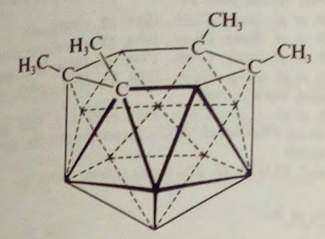
Lilac or yellow solids.

Cook, D.F. et al, Inorg. Chim. Acta, 1978, **31**, 59 (*synth, uv-vis*)

IC-006256

$C_8H_{23}B_{11}$

***C,C′,C″,C‴*-Tetramethyltetracarbaundecaborane(15), 10Cl**



M 238.1

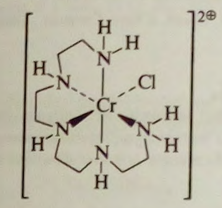
Tentative struct. shown. *nido*-. Air-stable colourless cryst. Sol. $CHCl_3$, hexane, C_6H_6. Mp 68°.

Hosmane, N.S. *et al, Inorg. Chem.*, 1980, **19**, 3482 (*synth, pmr, B-11 nmr, ms*)

IC-006257

$C_8H_{23}ClCrN_5^{2\oplus}$

Chloro(tetraethylenepentamine)chromium(*III*)(2+), 8Cl



M 276.7 (ion)

No crystallographic confirmation of isomeric octahedral form.

α,β-R-form

λ_{max} 375, 495 nm.

Dichloride: Synth. from $CrCl_3$ + ligand + Zn powder in anhyd. MeOH. Red violet cryst. (12*M* HCl/Me_2CO). Ir ν_{NH_2} 3200, 3150, 3070, 3015, δ_{NH_2} 1560 cm^{-1}.

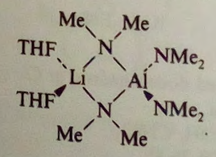
Tetrachlorozincate: Orange-red cryst.

House, D.A. *et al, Inorg. Chem.*, 1966, **5**, 2097; 1967, **6**, 272 (*synth, ir, uv-vis, cd*)

$C_8H_{24}AlN_4^{\ominus}$

IC-006258

Tetrakis(dimethylamido)aluminate(1−)



Li salt (*crystal*)

M 203.2 (ion)

Li salt: [114236-99-6].

$C_8H_{24}AlLiN_4$ M 210.2

Synth. from $LiAlH_4$ + Me_2NH. Made in var. ether solvs. Related compds. $LiAlH_{4-n}(NMe_2)_n$ also descr.

Li salt, bis-THF complex: [114237-01-3].

$C_{16}H_{40}AlLiN_4O_2$ M 354.4

Obt. from THF solns. of $Li[Al(NMe_2)_4]$. Colourless air- and moisture-sensitive plates (dibutyl ether). Loses THF in vacuum. Mp 50° dec.

Böck, St. *et al, Z. Naturforsch., B*, 1988, **43**, 53 (*synth, cryst struct*)

$C_8H_{24}B_2N_4$

IC-006259

Tetrakis(dimethylamino)diborane(4), 8Cl

Octamethyldiborane(4)*tetramine, 10Cl, 9Cl.*

Tetra(*dimethylamino*)*diboron*

[1630-79-1]

$(Me_2N)_2B{-}B(NMe_2)_2$

M 197.9

Liq., sensitive to moisture but stable at 200° in dry air. d_{22} 0.854. Mp −33°. Bp_9 86-93°, $Bp_{0.05}$ 42.5°. n_D^{21} 1.4679.

Brotherton, R.J. *et al, J. Am. Chem. Soc.*, 1960, **82**, 6242 (*synth*)

Nöth, H. *et al, Chem. Ber.*, 1961, **94**, 509 (*synth*)

Brubaker, G.L. *et al, Inorg. Chem.*, 1969, **8**, 2804 (*ms*)

Cetinkaya, B. *et al, J. Chem. Soc., Chem. Commun.*, 1971, 1370 (*pe*)

Nöth, H. *et al, Chem. Ber.*, 1973, **106**, 1145 (*nmr*)

Davidson, G. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 306 (*ir, raman*)

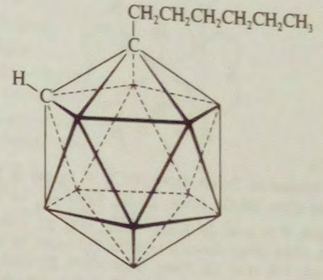
$C_8H_{24}B_{10}$

IC-006260

1-Hexyl-1,2-dicarbadodecaborane(12), 10Cl

1-Hexyl-o-carborane

[20740-05-0]



M 228.3

closo-. Rocket propellant burn rate modifier. Liq. Bp_{760} 326.7°, $Bp_{0.5}$ 102°. n_D^{25} 1.5211.

▷ HS9350000.

Heying, T.L. *et al, Inorg. Chem.*, 1963, **2**, 1089 (*synth*)

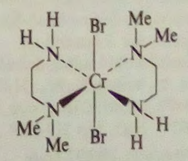
Fein, M.M. *et al, Inorg. Chem.*, 1963, **2**, 1115 (*synth*)

$C_8H_{24}Br_2CrN_4$

IC-006261

Dibromobis(*N,N*-dimethylethylenediamine)chromium(*II*), 8Cl

[33850-21-4]



M 388.1

Proposed struct. shown. Purple, air-sensitive solid. μ_{eff} = 4.93μ_B (300K). Corresp. iodide also reported.

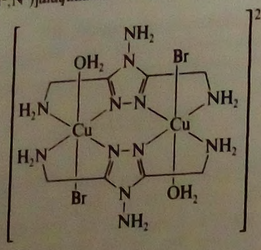
Larkworthy, L.F. *et al*, *J. Chem. Soc. A*, 1971, 2766 (*synth, props*)

IC-006262

$C_8H_{24}Br_2Cu_2N_{12}O_2^{2\oplus}$

Bis[μ-4-amino-3,5-bis(aminomethyl)-1,2,4-triazole-N^1,N^2,N^4]bis[aquabromocopper(*II*)](2+)

Bis[μ-(4-amino-4H-1,2,4-triazole-3,5-dimethanamine-N^1,N^2,N^4)]diaquadibromodicopper(2+)



M 607.2 (ion)

Dibromide: [119390-96-4].
Dark blue cryst. (aq. MeOH).

Koomen-van Oudenniel, W.M.E. *et al*, *Inorg. Chem.*, 1989, **28**, 1128 (*synth, cryst struct, ir, esr, magnetism*)

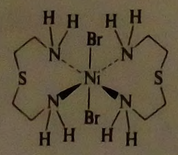
IC-006263

$C_8H_{24}Br_2N_4NiS_2$

Dibromobis(2,2′-diaminodiethylsulfide)nickel(*II*)

Dibromobis[2,2′-thiobis(ethanamine)-N,N′]nickel, 10CI

[67251-09-6]



M 458.9

trans-Octahedral. Synth. from $NiCl_2$ + ligand in MeOH. Violet cryst. (H_2O). Insol. EtOH, Et_2O. μ_{eff} = 2.98μ_B.

Kukushkin, Y.N. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 1294; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 712 (*synth, ir, struct*)
Ukraintsev, V.B. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 1836; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 1010 (*synth, ir*)

IC-006264

$C_8H_{24}Br_2O_4RuS_4$

Dibromotetrakis(dimethyl sulfoxide)ruthenium(*II*)

Dibromotetrakis[sulfinylbis[methane]]ruthenium(II), *9CI*

$RuBr_2[S(O)Me_2]_4$

M 573.4

Current interest in its antitumour props.

cis-form; all S-bonded DMSO-form [72937-89-4]
Dibromotetrakis[sulfinylbis[methane]-S]ruthenium(Ii), *9CI*

trans-form; all S-bonded DMSO-form [72904-46-2]
Dibromotetrakis[sulfinylbis[methane]-S]ruthenium(II), *9CI*
All DMSO ligands are *S*-bonded (cf. Dichlorotetrakis(dimethyl sulfoxide)ruthenium(*II*), IC-006280). Prepd. by boiling $RuBr_3.xH_2O$ in DMSO or by treating $[Ru(AsPh_3)_2(DMSO)Br_3]$ with DMSO. Yellow cryst. Sol. DMSO, H_2O. Mp 219-220°. Ir ν_{SO} 1080 cm^{-1}.

Perdeuterated trans-*form:* [50497-88-6].
$C_8Br_2D_{24}O_4RuS_4$ M 597.5

cis-form; mixed S,-O-bonded DMSO-form [72882-90-7]
Dibromo[sulfinylbis[methane]-O]tris[sulfinylbis[methane]-S] ruthenium(II), *9CI*
S-bonded DMSO ligands are *trans* to Br.

[50525-30-9]

Ruiz-Ramrez, L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1770 (*synth, pmr, ir*)
Ledlie, M.A. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1976, 1734 (*sulfide oxidation catalyst*)
Bora, T. *et al*, *Transition Met. Chem.*, 1978, **3**, 27 (*synth, ir*)
Barnes, J.R. *et al*, *J. Chem. Res.* (*S*), 1979, 350; *J. Chem. Res.* (*M*), 1979, 4301 (*synth, pmr, ir*)
Riley, D.P. *et al*, *Inorg. Chem.*, 1983, **22**, 1965 (*use*)
Oliver, J.P. *et al*, *Inorg. Chem.*, 1984, **23**, 156 (*cryst struct*)
Riley, D.P. *et al*, *Inorg. Chem.*, 1986, **25**, 1814, 1821 (*catalysis*)
Alessio, E. *et al*, *Inorg. Chem.*, 1988, **27**, 4099 (*synth, struct, pharmacol, trans forms*)
Alessio, E. *et al*, *J. Am. Chem. Soc.*, 1989, **111**, 7068 (*pharmacol*)
Sava, G. *et al*, *Pharmacol. Res. Commun.*, 1989, **21**, 617 (*pharmacol*)
Rudnitskaya, O.V. *et al*, *Zh. Neorg. Khim.*, 1989, **34**, 1761, 1780.

IC-006265

$C_8H_{24}CdO_4S_4^{2\oplus}$

Tetrakis(dimethyl sulfoxide)cadmium(2+)

Tetrakis[sulfinylbis[methane]-O]cadmium(2+)

$[Cd(O{=}SMe_2)_4]^{2\oplus}$

M 424.9 (ion)

Bis-tetrafluoroborate: [19973-68-3].
$C_8H_{24}B_2CdF_8O_4S_4$ M 598.5
Prepd. from hydrated $Cd(BF_4)_2$ + Me_2SO. White cryst. Stable in the absence of moisture.

Kutek, F., *Collect. Czech. Chem. Commun.*, 1968, **33**, 1930 (*synth, ir*)

IC-006266

$C_8H_{24}CeN_3O_{13}S_4$

Tetrakis(dimethyl sulfoxide)tris(nitrato)cerium(*III*)

Tris(nitrato-O,O′)tetrakis[sulfinylbis[methane]-O]cerium(III), *11CI*. *Cerium*(III) *nitrate tetrakis(dimethyl sulfoxide)*

[97057-46-0]

$Ce(NO_3)_3(O{=}SMe_2)_4$

M 638.6

Presumed 10-coord. White cryst. Sol. MeCN, Me_2CO, MeOH, DMSO. Mp 118°.

[20332-20-1]

Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581 (*synth*)
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

IC-006267

$C_8H_{24}CeP_4S_8^{\ominus}$

Tetrakis(dimethylphosphinodithioato-S,S')cerate(*III*)(1−)

Tetrakis(dimethyldithiophosphinato)cerate(III)(*1−*)

$[Ce(S_2PMe_2)_4]^{\ominus}$

M 640.8 (ion)

8-Coord. distorted dodecahedron at Ce.

Ph_4P salt: [66484-35-3].
Cryst. Sol. EtOH, $CHCl_3$.

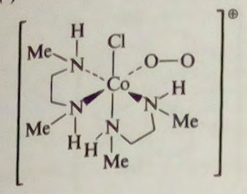
Ph_4As salt: [83709-36-8].
Colourless cryst. Sol. EtOH, CH_2Cl_2.

Pinkerton, A.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 85 (*synth, ir*)
Spiliadis, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 1809, 1815 (*synth, cryst struct, pmr, P-31 nmr*)

IC-006268

$C_8H_{24}ClCoN_4O_2^{\oplus}$

Chlorobis(N,N'-dimethylethylenediamine)(dioxygen) cobalt(*II*)(1+)



M 302.6 (ion)
Esr studies suggest a *cis*-octahedral struct. for the complex with monodentate O_2.

Perchlorate: Dark brown solid. Sol. EtOH.
▷ Potentially explosive.

Khare, G.P. *et al*, *Can. J. Chem.*, 1976, **54**, 342 (*synth, esr*)

IC-006269

$C_8H_{24}ClF_8N_4P_4Rh$

Chlorotetrakis[(dimethylamino)difluorophosphine] rhodium(*I*), 9CI

[50771-16-9]

$RhCl(PF_2NMe_2)_4$

M 590.5
Example of an aminophosphine complex. Yellow cryst. Mp 28-29°.

Bennett, M.A., *Aust. J. Chem.*, 1973, **26**, 2335 (*synth, ir, pmr, F-19 nmr*)

IC-006270

$C_8H_{24}ClN_4Ta$

Chlorotetrakis(dimethylamido)tantalum(*V*)

Chlorotetrakis(N-*methylmethanaminato*)*tantalum*(V), *11CI*

[82482-88-0]

$TaCl(NMe_2)_4$

M 392.7
Synth. from $Ta(NMe_2)_5$ and $[Ta(NMe_2)_3Cl_2]_2$ in hexane. Convenient starting material for synth. of compds. $RTa(NMe_2)_4$, R = alkyl. Yellow solid. Sol. hexane.

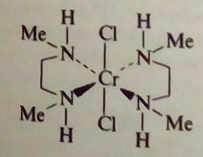
Chisholm, M.H. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 4879 (*synth, ir, pmr*)

IC-006271

$C_8H_{24}Cl_2CrN_4$

Dichlorobis(N,N'-dimethylethylenediamine)chromium(*II*), 8CI

[33850-20-3]



M 299.2
trans-Octahedral. Air-sensitive mauve solid. μ_{eff} = 4.81μ_B (90-300K).

Larkworthy, L.F. *et al*, *J. Chem. Soc. A*, 1971, 2766 (*synth, props*)

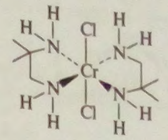
IC-006272

$C_8H_{24}Cl_2CrN_4$

Dichlorobis(2-methyl-1,2-propanediamine)chromium(*II*), 8CI

Dichlorobis(1,2-diamino-2-methylpropane)chromium(II)

[33847-25-5]



M 299.2
trans-Octahedral. Air-sensitive violet solid. μ_{eff} = 4.75μ_B (300K). Corresp. bromide and iodide also reported.

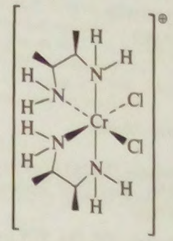
Larkworthy, L.F. *et al*, *J. Chem. Soc. A*, 1971, 2766 (*synth, props*)

IC-006273

$C_8H_{24}Cl_2CrN_4^{\oplus}$

Bis(2,3-butanediamine-N,N')dichlorochromium(*III*)(1+), 11CI, 10CI, 9CI

[53042-39-0]



meso,cis-form

M 299.2 (ion)

meso-cis-form
(RS,SR)-cis-*form*
Obt. using *meso*-form of ligand.

Perchlorate: [53042-40-3].
Pink-violet cryst + 0.5H_2O.

(±)-cis-form
(RS,RS)-cis-*form*
Obt. using racemic ligand.

Perchlorate: [53109-05-0].
Violet cryst. + H_2O.

(±)-trans-form
(RS,RS)-trans-*form*
Obt. using racemic ligand. Isom. to *cis*-form on heating.

Chloride: [79839-79-5].
Green cryst. + HCl + 2H_2O. Loses HCl at 55-80°, then 2H_2O at 100-140°. Turns violet at 180-240°, dec. above 240°.

Bromide: [79840-44-1].
Green cryst. + H_2O. Loses H_2O at 50-110°, turns violet at ~200°, dec. above 260°.

[53109-04-9]

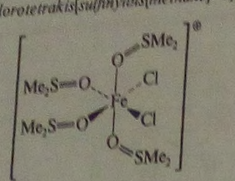
Madhusudan, C.P. *et al*, *Inorg. Chem.*, 1975, **14**, 82.
Tsuchiya, R. *et al*, *Inorg. Chem.*, 1982, **21**, 590 (*synth, trans form, dta*)

IC-006274

$C_8H_{24}Cl_2FeO_4S_4^{\oplus}$

Dichlorotetrakis(dimethyl sulfoxide-*O*)iron(*III*)(1+)

Dichlorotetrakis[sulfinylbis[methane]-O]iron(1+), 12Cl



cis-form

M 439.2 (ion)

Octahedral. Synth. from Fe + DMSO in CCl_4 produces mixtures of *cis* and *trans* products, as Cl or $FeCl_4$ salts. Catalyst for telomerisation of olefins with CCl_4.

cis-form

Chloride: [64658-74-8]. *Ferric chloride tetrakis(dimethyl sulfoxide)*

$C_8H_{24}Cl_3FeO_4S_4$ M 474.7

Tetrachloroferrate(II) (*2:1*): [53862-27-4].

$C_{16}H_{48}Cl_8Fe_3O_8S_8$ M 1076.2

Yellow.

Tetrachloroferrate(III): [15337-31-2].

$C_8H_{24}Cl_6Fe_2O_4S_4$ M 636.9

Yellow.

trans-form

Chloride: [54010-41-2].

Tetrachloroferrate(III): *Ferric chloride bis(dimethylsulfoxide)*

Obt. from $FeCl_3$ + anhydrous DMSO. Yellow cryst. (EtOH). Sol. DMSO, EtOH. Subl. 190°. Previously formulated as $FeCl_3.2DMSO$.

Bennett, M.J. *et al*, *Nature* (*London*), 1966, **212**, 5059 (*synth, cryst struct, trans-form*)

Bennett, M.J. *et al*, *Acta Crystallogr.*, 1967, **23**, 581 (*cryst struct, trans-form*)

Ponomarev, V.I. *et al*, *Koord. Khim.*, 1977, **3**, 1256; 1982, **8**, 98 (*synth, cryst struct, cis-form*)

Lavrent'ev, I.P. *et al*, *Koord. Khim.*, 1979, **5**, 1484 (*synth, cryst struct, mössbauer*)

Lavrent'ev, I.P. *et al*, *Transition Met. Chem.*, 1980, **5**, 193 (*synth, mössbauer*)

Kutaigorodskii, A.N. *et al*, *Zh. Fiz. Khim.*, 1982, **56**, 969 (*synth, nmr*)

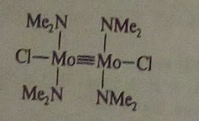
IC-006275

$C_8H_{24}Cl_2Mo_2N_4$

Dichlorotetrakis(dimethylamido)dimolybdenum(*III*)

Dichlorotetrakis(N-*methylmethanaminato*)*dimolybdenum*(III), *11Cl*

[63301-82-6]



M 439.0

Triply bonded species in a staggered ethane-like config. Interatomic distance: Mo≡Mo 220.1 pm. Synth. from $Mo_2(NMe_2)_6$ and Me_3SiCl at r.t. Important starting material for dinuclear Mo complexes. V. air- and moisture-sensitive; golden-yellow cryst. (by subl. or hexane or toluene). Sol. hydrocarbon solvs. $Subl._{0.0001}$ 100-120°. Dec. in THF or Et_2O. Diamagnetic.

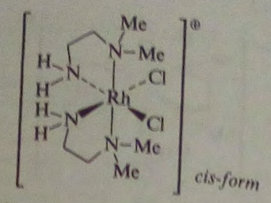
Akiyama, M. *et al*, *Inorg. Chem.*, 1977, **16**, 2407 (*cryst struct, synth, pmr, ir, ms*)

Inorg. Synth., 1982, **21**, 51 (*synth, reactions*)

$C_8H_{24}Cl_2N_4Rh^{\oplus}$

IC-006276

Dichlorobis(*N*,*N*-dimethylethylenediamine)rhodium(*III*)(1+)



cis-form

M 350.1 (ion)

cis and *trans* forms do not interconvert.

cis-form

Early literature incorrectly assigned this *trans*. Struct. comprises only one of 3 possible *cis*-isomers.

Perchlorate: [60133-92-8].

Feathery yellow cryst. (hot H_2O).

all-trans-form

Iodide:

$C_8H_{24}Cl_2IN_4Rh$ M 477.0

Bright yellow cryst. (EtOH aq.).

Perchlorate: [60133-88-2].

Orange-yellow cryst. (hot H_2O).

Hancock, M.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 931 (*synth, pmr, uv*)

IC-006277

$C_8H_{24}Cl_2N_4W_2$

Dichlorotetrakis(dimethylamido)ditungsten(*III*)

Dichlorotetrakis(N-*methylmethanaminato*)*ditungsten, 11Cl, 10Cl*

[63301-81-5]

$(Me_2N)_2WCl{\equiv}WCl(NMe_2)_2$

M 614.9

W≡W 228.5 pm. Synth. from $W_2(NMe_2)_6$ + $2Me_3SiCl$ in toluene. Starting material for many W—W compds. Volatile, v. air-sensitive yellow cryst. Sol. hydrocarbons. Dec. in Et_2O, THF. $Subl._{0.001}$ 100-120°.

Akiyama, M. *et al*, *Inorg. Chem.*, 1977, **16**, 2407 (*cryst struct, synth, pmr, ir, ms*)

Chisholm, M.H., *Organometallics*, 1986, **5**, 185 (*reactions*)

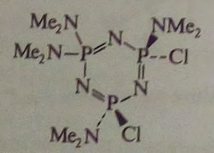
IC-006278

$C_8H_{24}Cl_2N_7P_3$

2,4-Dichloro-2,4,5,6-tetrakis(dimethylamino)-2,2,4,4,6,6-hexahydro-1,3,5,2,4,6-triazatriphosphorine, 9Cl

2,4-Dichloro-2,4,6,6-tetrakis(dimethylamino)-2,2,4,4,6,6-hexahydrocyclotriphosphazene. 2,4-Dichloro-2,4,6,6-tetrakis(dimethylamino)-2λ⁵,4λ⁵,6λ⁵-cyclotriphosphaza-1,3,5-triene. 2,4-Dichloro-2,4,6,6-tetrakis(dimethylamino)-1,3,5,2λ⁵,4λ⁵,6λ⁵-triazatriphosphinine

[22514-10-9]



(*4RS,6RS*)-*form*

M 382.1

cis- and *trans*-forms equilibrate in soln.

(4RS,6RS)-form [5591-07-1]

trans-*form*

Cryst. (pet. ether). Mp 72°. $Bp._{0.01}$ 40° subl.

(4RS,6SR)-form [963-05-3]

cis-form

Cryst. (pet. ether). Mp 104°.

Keat, R. *et al*, *J. Chem. Soc.*, 1965, 2215 (*synth, struct*)

Strahlberg, R. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2005 (*ir, raman*)

Green, B. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 3687 (*pmr, ir, glc*)

Dagleish, W.H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 309 (*nqr*)

Keat, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1582 (*P-31 nmr*)

Goldschmidt, J.M.E. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **42**, 618 (*synth*)

Friedmann, N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 103 (*props*)

Katti, K.V. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 285 (*glc*)

IC-006279

$C_8H_{24}Cl_2NiO_4$

Dichlorotetrakis(ethanol)nickel(*II*), 9Cl

Dichlorotetrakis(ethyl alcohol)nickel. Nickel(II) *chloride tetrakis(ethanol)*

[15696-86-3]

$NiCl_2(EtOH)_4$

M 313.8

trans-Octahedral. Pale-green hygroscopic needles; loses EtOH on heating. V. sol. alcohols, esters, THF. Insol. hydrocarbons, Et_2O, CH_2Cl_2.

Inorg. Synth., 1971, **13**, 154 (*synth, props*)

Bkouche-Waksman, I., *J. Inorg. Nucl. Chem.*, 1976, **38**, 1871 (*cryst struct*)

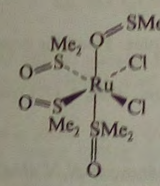
IC-006280

$C_8H_{24}Cl_2O_4RuS_4$

Dichlorotetrakis(dimethyl sulfoxide)ruthenium(*II*)

Dichlorotetrakis[sulfinylbis[methane]]ruthenium(II), *9Cl*

[11070-19-2]



cis-form

M 484.5

Many isomers exist; the principal ones are detailed here. Prepd. by heating $RuCl_3.xH_2O$ in boiling DMSO. Sol. DMSO, H_2O.

▷VM2651450.

cis-form, with three S-bonded and one O-bonded DMSO ligands-form [59091-96-2]

Dichloro[sulfinylbis[methane]-O]tris[sulfinylbis[methane]-S] ruthenium, 9Cl

Contains *fac* config. of 3*S*-bonded DMSO ligands, a single *O*-bonded DMSO ligand, and 2 *cis*-chlorides. Yellow solid. Sol. DMSO, H_2O. Mp 193° dec. Ir $\nu_{SO\text{-}bonded}$ 1120, 1090; $\nu_{SOO\text{-}bonded}$ 915; $\nu_{Ru\text{-}Cl}$ 258, 248 cm^{-1}. $Ru{-}S_{trans\,to\,Cl}$ 227.7; $Ru{-}S_{trans\,to\,O}$ 225.2; Ru—O 214.2; Ru—Cl 243.5; $S{-}O_{S\text{-}bonded}$ 148.4; $S{-}O_{O\text{-}bonded}$ 155.7 pm.

cis-form, with four S-bonded DMSO ligands-form [64376-67-6]

Dichlorotetrakis[sulfinylbis[methane]-S]ruthenium, 9Cl

Sol. DMSO, H_2O.

trans-form, with three S-bonded and one O-bonded DMSO ligands-form [75766-08-4]

Dichloro[sulfinylbis[methane]-O]tris[sulfinylbis[methane]-S] ruthenium, 9Cl

Sol. DMSO, H_2O.

trans-form, with four S-bonded DMSO ligands-form [72904-47-3]

It is possible that not all the DMSO ligands are *S*-bonded; the struct. remains unproven. Red solid. Mp 120° dec.

Mono-O, tris-S-bonded-form [41290-68-0]

Dichloro[sulfinylbis[methane]-O]tris[sulfinylbis[methane]-S] ruthenium, 9Cl

Sol. DMSO, H_2O.

Bis-O, bis-S-bonded-form [61779-29-1]

Dichlorobis[sulfinylbis[methane]-O]bis[sulfinylbis[methane]-S]ruthenium, 9Cl

Sol. DMSO, H_2O.

James, B.R. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 781 (*synth, ir*)

Evans, I.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 204 (*synth, ir, uv, reactions*)

McMillan, R.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1066 (*catalysis*)

Mercer, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 2480 (*cryst struct*)

James, B.R. *et al*, *J. Mol. Catal.*, 1975/76, **1**, 439 (*catalysis*)

Bora, T. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 1815 (*synth, thermochem*)

Giraldi, T. *et al*, *Cancer Res.*, 1977, **37**, 2662 (*antitumour activity*)

Klugmann, P.B. *et al*, *Pharmacol. Res. Commun.*, 1977, **9**, 149 (*antitumour activity*)

Barnes, J.R. *et al*, *J. Chem. Res.* (*S*), 1979, 350; *J. Chem. Res.* (*M*), 1979, 4301 (*synth, pmr, ir*)

Heath, G.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 2429 (*synth, ir, cmr, pmr, electrochem*)

IC-006281

$C_8H_{24}Cl_2O_4V$

Dichlorotetrakis(ethanol)vanadium(*II*), 11Cl

Vanadium(II) *chloride tetrakis(ethanol)*

[86526-08-1]

$VCl_2(EtOH)_4$

M 306.1

Octahedral; exact geometry unknown. Synth. from $VCl_2.4H_2O$ in EtOH and excess ethyl orthoformate. Pale blue solid. Paramagnetic, μ_{eff} = 3.68 (295K), $3.56\mu_B$ (90K), θ = 8K.

Larkworthy, L.F. *et al*, *Inorg. Chim. Acta*, 1983, **71**, 81 (*synth, uv-vis, magnetism*)

IC-006282

$C_8H_{24}Cl_2O_4V^{\oplus}$

Dichlorotetrakis(ethanol)vanadium(*III*)(1+), 10Cl

$[VCl_2(EtOH)_4]^{\oplus}$

M 306.1 (ion)

cis-Octahedral. Similar compounds with other alcohols are known.

Chloride: [25992-90-9].

$C_8H_{24}Cl_2O_4V$ M 341.5

Synth. by dissolving VCl_3 in EtOH, cooling to −40° and saturating with HCl. Green solid; in soln. the compd. both fluoresces and undergoes photoreduction to V(*II*) simultaneously. Paramagnetic, μ_{eff} = $2.73\mu_B$ (295K) and $2.54\mu_B$ (86K).

[73494-79-8]

Casey, A.T. *et al*, *Inorg. Chem.*, 1969, **8**, 1216 (*synth, uv-vis, ir, magnetism*)

Doi, Y. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3243 (*fluorescence, photoreduction*)

IC-006283

$C_8H_{24}Cl_2RuS_4$

Dichlorotetrakis[thiobis[methane]]ruthenium

Dichlorotetrakis(dimethyl sulfide)ruthenium(II)

[32648-28-5]

$RuCl_2(SMe_2)_4$

M 420.5

trans-Octahedral. Prepd. as a by-product in the reaction between $RuCl_3.xH_2O$ and SMe_2 in MeOH. Yellow solid. Mp ~120° dec.

[99033-10-0]

Chatt, J. *et al*, *J. Chem. Soc. A*, 1971, 1380 (*synth*)
Riley, D.P. *et al*, *Chem. Ind. (Dekker)*, 1985, **22**, 281; *CA*, **104**, 75876 (*catalysis*)
Riley, D.P. *et al*, *Inorg. Chem.*, 1986, **25**, 1814 (*oxidation, catalysis*)

IC-006284

$C_8H_{24}Cl_3O_4S_4Sc$

Trichlorotetrakis(dimethyl sulfoxide)scandium(*III*)

Dichlorotetrakis(methylsulfoxide)scandium(1+) chloride, 8CI

[20303-54-2]

$(Me_2SO)_4ScCl_3$

M 463.8

Possibly formulated as $Sc(OSMe_2)_4Cl_2^{\oplus}Cl^{\ominus}$. Colourless cryst. Sol. Me_2CO, DMSO.

Kůtek, F. *et al*, *Collect. Czech. Chem. Commun.*, 1968, **33**, 296 (*synth, ir*)

IC-006285

$C_8H_{24}Cl_4Ga_2N_2Si_2$

Tetradichlorobis[methyl(trimethylsilyl)amido]digallium

Tetrachlorobis[μ-(N,1,1,1-tetramethylsilanaminato)] digallium, 11CI

As Tetrabromobis(trimethylsilylamido)digallium, IC-005433 with

R = Me, X = Cl

M 485.7

Synth. from $GaCl_3$ and $(Me_3Si)_2NMe$ in Et_2O.

cis-form [93780-86-0]

Not isol. Detected in soln. by nmr.

trans-form [93683-64-8]

Colourless air and moisture sensitive cryst. (by subl.). Sol. CH_2Cl_2, toluene. Mp 164-171°.

Monomer: Dichloro[methyl(trimethylsilyl)amido]gallium
$C_4H_{12}Cl_2GaNSi$ M 242.8
Not known.

Nult, W.R. *et al*, *Inorg. Chem.*, 1985, **24**, 159 (*synth, pmr, cmr, ir, cryst struct*)

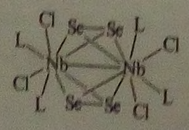
IC-006286

$C_8H_{24}Cl_4Nb_2S_4Se_4$

Tetrachlorobis[μ-(diselenium-*Se,Se':Se,Se'*)] tetrakis(dimethyl sulfide)diniobium(*IV*)

Tetrachlorotetrakis(dimethyl sulfide)bis[μ-(diseleno)] diniobium(IV). *Di(μ-diselenido)bis[dichlorobis(dimethyl sulfide)niobium*(IV)]

[92181-24-3]



L = SMe_2

M 892.0

Synth. from $NbCl_3Se$ + neat Me_2S. Red cryst. (CS_2).

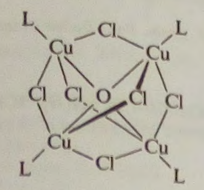
Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 1087 (*synth, cryst struct*)

$C_8H_{24}Cl_6Cu_4O_5S_4$ IC-006287

μ$_4$-Oxohexa-μ-chloro-tetrakis(dimethyl sulfoxide) tetracopper(*II*)

Hexa-μ-chloro-μ$_4$-oxotetrakis[sulfinylbis[methane]-O] tetracopper, 12CI

[121480-91-9]



L = $OSMe_2$

M 795.4

Tetrahedron of Cu_4 with central oxygen atom. Orange cryst. + DMSO. Sol. DMSO, EtOH; Insol. hexane.

Brownstein, S. *et al*, *Can. J. Chem.*, 1989, **67**, 551 (*synth, cryst struct*)

IC-006288

$C_8H_{24}CrI_2O_4S_4$

Diiodotetrakis(dimethyl sulfoxide)chromium(*II*)

Diiodotetrakis(methyl sulfoxide)chromium. Chromium(II) *iodide tetrakis(dimethyl sulfoxide)*

$CrI_2(O{=}SMe_2)_4$

M 618.3

Distorted octahedral complex. Pale blue cryst. (EtOH). μ_{eff} = 4.95μ_B (293K).

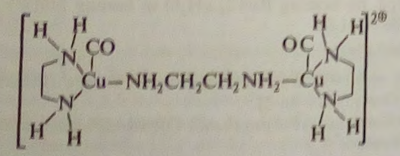
Holah, D.G. *et al*, *Inorg. Chem.*, 1966, **4**, 1721 (*synth, uv, ir*)

IC-006289

$C_8H_{24}Cu_2N_6O_2^{2\oplus}$

Dicarbonyl[μ-(1,2-ethanediamine-*N,N'*)]bis(1,2-ethanediamine-*N,N'*)dicopper(2+), 10CI

[69683-75-6]



M 363.4 (ion)

Bis(tetraphenylborate):
$C_{56}H_{64}B_2Cu_2N_6O_2$ M 1001.8
Cryst. (MeOH). Mp 80° dec. Sensitive to moisture, rel. high thermal stability.

Pasquali, M. *et al*, *Inorg. Chem.*, 1980, **19**, 1191 (*synth, cryst struct*)

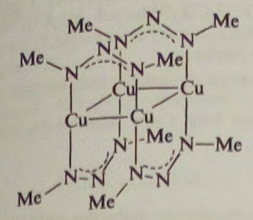
IC-006290

$C_8H_{24}Cu_4N_{12}$

Tetrakis[μ-(1,3-dimethyltriazenato)]tetracopper(*I*), 8CI

Tetrakis[1,3-dimethyltriazenocopper(I)]

[21315-81-1]



M 542.5

Planar copper tetramer with Cu—Cu 267 pm. Yellow cryst. (pet. ether). Sol. Et_2O, $CHCl_3$, insol. H_2O. Mp 185-186°.

Monomer: 1,3-Dimethyltriazenatocopper
$C_2H_6CuN_3$ M 135.6
Unknown.

Dimroth, E.O., *Chem. Ber.*, 1905, **38**, 670; 1906, **39**, 3905 (*synth*)
Harris, C.M. *et al*, *J. Chem. Soc.*, 1959, 3728 (*synth*)
O'Connor, J.E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1968, 445 (*cryst struct*)
Kuyper, T. *et al*, *J. Organomet. Chem.*, 1975, **96**, 289 (*props*)

IC-006291

$C_8H_{24}EuN_3O_{13}S_4$

Tetrakis(dimethyl sulfoxide)tris(nitrato)europium(*III*)

Tris(nitrato-O,O')tetrakis[sulfinylbis[methane]-O] europium(III), *9CI. Europium*(III) *nitrate tris(dimethyl sulfoxide)*

[81654-67-3]

$Eu(NO_3)_3(O{=}SMe_2)_4$

M 650.5

10-Coordinate with all nitrates bidentate. White cryst. Sol. MeCN, Me_2CO, MeOH, DMSO.

[63796-63-4]

Tsaryuk, V.I. *et al*, *Koord. Khim.*, 1977, **3**, 829; *Sov. J. Coord. Chem. (Engl. Transl.)*, 1977, **3**, 640 (*ir, luminescence*)
Lin, Y. *et al*, *Wuli Xuebao*, 1981, **30**, 1586; *CA*, **96**, 191071 (*cryst struct*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581 (*synth*)
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

IC-006292

$C_8H_{24}F_8N_4NiP_4$

Tetrakis(dimethylaminodifluorophosphine)nickel(0)

Tetrakis(dimethylphosphoramidous difluoride-P)nickel, 9CI

[15053-92-6]

$Ni(PF_2NMe_2)_4$

M 510.8

Probably approx. T_d at Ni. Air stable cryst. (Et_2O). Mp 110-111°.

Kruck, T. *et al*, *Chem. Ber.*, 1974, **107**, 2145, 2156 (*synth, ir, pmr, ms*)
Severiault, J.-M. *et al*, *J. Fluorine Chem.*, 1974, **4**, 159 (*props*)
King, R.B. *et al*, *Inorg. Chem.*, 1979, **18**, 364 (*synth, pmr, ms*)
Severson, S.J. *et al*, *Inorg. Chem.*, 1983, **22**, 3833 (*synth*)

IC-006293

$C_8H_{24}F_8N_4P_4Rh^{\ominus}$

Tetrakis(dimethylphosphoramidous difluoride-*P*) rhodate(1−), 9CI

Tetrakis(dimethylaminodifluorophosphine)rhodate(−1)

$[Rh(PF_2NMe_2)_4]^{\ominus}$

M 555.0 (ion)

Ligand probably binds through P.

K salt: [39733-65-8].
Off-white solid. Sol. C_6H_6.

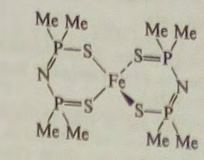
Clement, D.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 195 (*synth, ir, F-19 nmr*)

IC-006294

$C_8H_{24}FeN_2P_4S_4$

Bis[[iminobis[dimethylphosphine sulfidato]](1−)]iron(*II*)

[29950-57-0]



M 456.2

Tetrahedral at Fe. Synth. from $(Me_2PS)_2NH$ + NaOMe in MeOH + $[FeCl_4]^{2\ominus}$. Colourless cryst. (CH_2Cl_2/heptane). Oxidises readily in soln. and solid. Sol. CH_2Cl_2, MeOH. Subl. 186-188°. μ_{eff} = 5.25μ_B.

Churchill, M.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 703 (*struct*)
Davison, A. *et al*, *Inorg. Chem.*, 1971, **10**, 837 (*synth, uv, pmr*)

IC-006295

$C_8H_{24}GaN_4^{\ominus}$

Tetrakis(dimethylamido)gallate(1−)

Tetrakis(N-*methylmethanaminato) gallate*(1−)

$[Ga(NMe_2)_4]^{\ominus}$

M 246.0 (ion)

Li salt: [57731-41-6].
$C_8H_{24}GaLiN_4$ M 252.9
Synth. from $LiNMe_2$ + $GaCl_3$ in Et_2O. Colourless air and moisture sensitive solid (C_6H_6/pentane).

Nöth, H. *et al*, *Z. Naturforsch., B*, 1975, **30**, 681 (*synth, ir, pmr*)

IC-006296

$C_8H_{24}GdN_3O_{19}S_4$

Tetrakis(dimethyl sulfoxide)tris(nitrato)gadolinium(*III*)

Tris(nitrato-O,O')tetrakis[sulfinylbis[methane]-O] gadolinium(III), *11CI. Gadolinium*(III) *nitrate tetrakis(dimethyl sulfoxide)*

[97057-47-1]

$Gd(NO_3)_3(O{=}SMe_2)_4$

M 655.8

Probably 10-coordinate with all nitrates bidentate. White cryst. Sol. MeCN, Me_2CO, MeOH, DMSO. Mp 104°.

[12107-83-4, 18253-75-3]

Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth, ir*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581 (*synth*)
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

IC-006297

$C_8H_{24}GeN_4$

Tetrakis(dimethylamino)germane

Octamethylgermanetetramine

[7344-40-3]

$Ge(NMe_2)_4$

M 248.9

d_4^{25} 1.069. Mp 14°. Bp 205°, Bp_{15} 87-89°.
Anderson, H.H., *J. Am. Chem. Soc.*, 1952, **74**, 1421 (*synth*)
Buerger, H. *et al*, *Inorg. Nucl. Chem. Lett.*, 1966, **2**, 209 (*ir*)
Schaeffer, C.D. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 3659 (*cmr*)

IC-006298

$C_8H_{24}I_2InO_2S_4^{\oplus}$
Tetrakis(dimethyl sulfoxide)diiodoindium(1+)
Diiodotetrakis(methyl sulfoxide)indium(1+), 9CI

cis-$[InI_2(OSMe_2)_4]^{\oplus}$

M 681.1 (ion)
Tetraiodoindate(1−): [30420-18-9]. *Indium*(III) *iodide-tetrakis(dimethyl sulfoxide)*
$C_8H_{24}I_4In_2O_4S_8$ M 1303.6
Yellow cryst. (EtOH). Sol. EtOH, $MeNO_2$; spar. sol. Et_2O, C_6H_6. Dec. > 175°. Previously formulated as neutral $InI_3(O{=}SMe_2)_2$.
Curry, A.J. *et al*, *J. Chem. Soc. A*, 1966, 1081 (*synth, props*)
Curry, A.J. *et al*, *Can. J. Chem.*, 1970, **48**, 482 (*ir, raman*)
Einstein, F.W.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 1182 (*cryst struct, raman*)

IC-006299

$C_8H_{24}I_2O_4RuS_4$
Tetrakis(dimethyl sulfoxide-*S*)diiodoruthenium(*II*)
Diiodotetrakis[sulfinylbis[methane]-S]ruthenium(II), *9CI*
[12191?-86-0]

$RuI_2[S(O)Me_2]_4$

M 667.4
trans-Octahedral; all DMSO ligands are *S*-bonded (*cf.* Dichlorotetrakis(dimethyl sulfoxide)ruthenium(*II*), IC-006280). Brown solid. Sol. DMSO, H_2O.
[86745-74-2, 72907-35-8]
Bora, T. *et al*, *Transition Met. Chem.*, 1978, **3**, 27 (*synth, ir*)
Barnes, J.R. *et al*, *J. Chem. Res. (S)*, 1979, 350; *J. Chem. Res. (M)*, 1979, 4301 (*synth, pmr, ir*)
Riley, D.P. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 3179 (*oxid/cysis*)
Sarma, U.C. *et al*, *Polyhedron*, 1988, **7**, 2627 (*synth*)
Sava, G. *et al*, *Pharmacol. Rev.*, 1989, **21**, 617 (*biochem, antitumour agent*)

$C_8H_{24}LaN_3O_{13}S_4$ IC-006300
Tetrakis(dimethyl sulfoxide)tris(nitrato)lanthanum
Tetrakis(dimethyl sulfoxide)lanthanum(III) *nitrate. Lanthanum*(III) *nitrate tetrakis(dimethyl sulfoxide)*
[32409-39-5]

$La(NO_3)_3(O{=}SMe_2)_4$

M 637.4
10-Coordinate with bidentate nitrates. White cryst. Sol. MeCN, Me_2CO, MeOH, DMSO. Mp 116°.
Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth*)
Bhandary, K.K. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 1093 (*cryst struct*)
Kawano, Y. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 701 (*ir, raman*)
James, B.R. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 577 (*ir*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581.
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

$C_8H_{24}MnO_6^{2\oplus}$ IC-006301
Diaquabis(1,2-dimethoxyethane-*O,O'*)manganese(*II*)(2+), 9CI

$[Mn(OH_2)_2(MeOCH_2CH_2OMe)_2]^{2\oplus}$

M 271.2 (ion)
Distorted octahedral cation; detailed geometry not known.
Diperchlorate: [38549-33-6].
Prepared from $Mn(ClO_4)_2{\cdot}4H_2O$ and $MeOCH_2CH_2OMe$ in the presence of $HC(OEt)_3$/EtOH. Light tan cryst. Insol. $MeOCH_2CH_2OMe$; sol. Me_2CO, $MeNO_2$; μ_{eff} = 6.15μ_B (300K).
▷ Potentially explosive.
Karayannis, N.M., *Inorg. Chem.*, 1972, **11**, 2330 (*synth, ir, uv, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 141 (*rev, bibl*)

$C_8H_{24}MoN_4$ IC-006302
Tetrakis(dimethylamido)molybdenum(*IV*)
Molybdenum(IV) *dimethylamide. Tetrakis(N-methyldimethanaminato)molybdenum*(IV), *11CI*
[33851-46-6]

$Mo(NMe_2)_4$

M 272.2
Tetrahedral at Mo. Synth. from $MoCl_5$ and $LiNMe_2$. Extremely volatile purple cryst. Mp ~ 50°.
[100207-68-9]
Bradley, D.C. *et al*, *J. Chem. Soc. A*, 1971, 2741 (*synth, props, ir, nmr, ms, uv*)
Chisholm, M.H. *et al*, *Inorg. Chem.*, 1978, **17**, 1329 (*cryst struct*)
Beach, D.B. *et al*, *Inorg. Chem.*, 1986, **25**, 875 (*pe*)

$C_8H_{24}Mo_3O_{13}S_4$ IC-006303
Di(μ-oxo)dioxobis[bis(dimethyl sulfoxide)dioxomolybdenum(*VI*)]molybdenum(*VI*)
Tetrakis(dimethyl sulfoxide)tri-μ-oxohexaoxotrimolybdenum. Di-μ-oxoheptaoxotetrakis[sulfinylbis[methane]-O]trimolybdenum, 11CI
[86086-48-8]

$[\text{-O-}MoO_2(DMSO)_2\text{-O-}MoO_2\text{-O-}MoO_2(DMSO)_2\text{-}]_n$

M 744.3
Struct. comprises infinite chains of octahedral and tetrahedral Mo. Obt. in slightly differing forms according to synthetic conditions. Colourless parallelepiped cryst.
McCarron, E.M. *et al*, *J. Chem. Soc., Chem. Commun.*, 1983, 90 (*cryst struct, synth*)

$C_8H_{24}N_3NdO_{13}S_4$ IC-006304
Tetrakis(dimethyl sulfoxide)tris(nitrato)neodymium
Tetrakis(dimethyl sulfoxide)neodymium nitrate. Neodymium(III) *nitrate tetrakis(dimethyl sulfoxide)*
[36606-63-0]

$Nd(NO_3)_3(O{=}SMe_2)_4$

M 642.7
10-Coordinate with bidentate nitrates. Pink cryst. Sol. MeCN, Me_2CO, MeOH. Mp 114°.
Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*ir*)
Aslanov, L.A. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1972, **13**, 610 (*cryst struct*)
Kawano, Y. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 701 (*ir, raman*)
James, B.R. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 577 (*ir*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581.
Su, Q. *et al*, *Zhongguo Xitu Xuebao*, 1985, **3**, 33; *CA*, 1986, **104**, 13818 (*magnetism*)

Hanuza, J. *et al*, *Spectrochim. Acta, Part A*, 1986, **42**, 1089 (*ir, raman, uv-vis, luminescence*)
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

IC-006305

$C_8H_{24}N_3O_{13}PrS_4$
Tetrakis(dimethyl sulfoxide)tris(nitrato)praseodymium(*III*)
Tris(nitrato-O,O')tetrakis[sulfinylbis[methane]-O]praseodymium(III), *9CI. Praseodymium*(III) *nitrate tetrakis(dimethyl sulfoxide)*
[38058-07-6]

$Pr(NO_3)_3(O{=}SMe_2)_4$

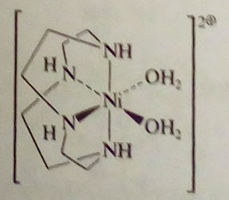
M 639.4
10-Coordinate, all nitrates bidentate. Green cryst. Sol. MeCN, Me_2CO, MeOH, DMSO. Mp 115°.
[12107-56-7, 90579-08-9]
Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth*)
Aslanov, L.A. *et al*, *Zh. Strukt. Khim.*, 1972, **12**, 1112 (*cryst struct*)
Lin, Y. *et al*, *Huaxue Xuebao*, 1984, **42**, 272; *CA*, **101**, 15367 (*cryst struct*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, 1985, **103**, 31581 (*synth*)
Bao, F. *et al*, *Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

$C_8H_{24}N_3O_{13}S_4Sm$ IC-006306
Tetrakis(dimethyl sulfoxide)tris(nitrato)samarium(*III*)
Tris(nitrato-O,O')tetrakis[sulfinylbis[methane]-O]samarium(III), *11CI. Samarium*(III) *nitrate tetrakis(dimethyl sulfoxide)*
[37425-82-8]

$Sm(NO_3)_3(O{=}SMe_2)_4$

M 648.9
Assumed 10-coordinate as isomorphous with La analogue. Pale yellow cryst. Sol. MeCN, Me_2CO, MeOH, DMSO. Mp 104°.
[12107-87-8, 18079-15-7]
Ramalingam, S.K. *et al*, *J. Inorg. Nucl. Chem.*, 1967, **29**, 1763 (*synth*)
Bhandary, K.K. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 1997 (*struct*)
Su, Q. *et al*, *Yingyong Huaxue*, 1985, **2**, 1; *CA*, **103**, 31581 (*synth*)
Bao, F. *et al*, *Wuli Huaxue Xuebao*, 1986, **2**, 321; *CA*, **105**, 142484 (*ir, raman*)

$C_8H_{24}N_4NiO_2^{2\oplus}$ IC-006307
Diaqua(1,4,7,10-tetraazacyclododecane-N^1,N^4,N^7,N^{10})nickel(*II*)(2+)



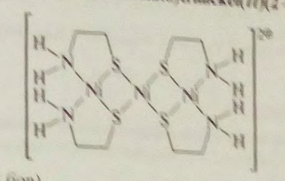
M 266.9 (ion)
cis-Octahedral cation. Simple example of folded macrocyclic ligand leaving two *cis*-positions vacant.
Diperchlorate: Purple cryst. + H_2O (EtOH aq.).
▷ Potentially explosive.
Scott, B. *et al*, *J. Coord. Chem.*, 1990, **21**, 307 (*synth, cryst struct*)

$C_8H_{24}N_4NiO_6^{2\oplus}$ IC-006308
Tetrakis(acetamide)diaquanickel(*II*)(2+), 9CI

$[Ni(OH_2)_2(H_3CCONH_2)_4]^{2\oplus}$

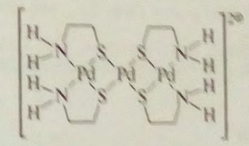
M 330.9 (ion)
Amide coordinates through O. Octahedral.
***trans*-form**
Dichloride: [36445-01-9].
$C_8H_{28}Cl_2N_4NiO_4$ M 401.8
Hygroscopic cryst. (EtOH/MeOH). Sol. EtOH. Ir ν_{CO} 1672; ν_{NH} 1586 cm^{-1} (KBr).
[41930-74-9]
Stone, M.E. *et al*, *J. Chem. Soc. A*, 1971, 3632 (*cryst struct*)
Stone, M.E. *et al*, *Can. J. Chem.*, 1973, **51**, 1280 (*synth, ir, uv*)

$C_8H_{24}N_4Ni_3S_4^{2\oplus}$ IC-006309
Tetrakis(2-aminoethanethiolato)trinickel(*II*)(2+), 8CI



M 480.6 (ion)
Square planar struct. for each Ni. Also known with other metals in centre position.
Dichloride: [29993-19-9].
Dark green plates. Sol. MeOH, EtOH.
Busch, D.H. *et al*, *Inorg. Chem.*, 1962, **1**, 872, 878 (*synth, props*)
Wei, C.H. *et al*, *Inorg. Chem.*, 1970, **9**, 1878 (*cryst struct*)

$C_8H_{24}N_4Pd_3S_4^{2\oplus}$ IC-006310
Tetrakis[μ-(2-aminoethanethiolato-N,S:S)]tripalladium(*II*)(2+), 10CI



M 623.8 (ion)
Linear trimer with square planar Pd. Synth. from Tetrachloropalladate(*II*)(2−), IC-017115 + $[Pd(NH_2CH_2CH_2S)_2]$. Ni, Se and mixed metal analogues known.
Dichloride: [63287-50-3].
Yellow solid (EtOH aq.). Sol. H_2O.
Jicha, D.C. *et al*, *Inorg. Chem.*, 1962, **1**, 872, 878 (*synth, props*)
Reichert, R. *et al*, *Helv. Chim. Acta*, 1977, **60**, 722.

$C_8H_{24}N_4Si$ IC-006311
Tetrakis(dimethylamino)silane
Octamethylsilanetetramine, 9CI, 8CI
[1624-01-7]

$Si(NMe_2)_4$

M 204.3
Cocatalyst for alkene polymerisation. d 0.973, d 0.885. Mp −2°. Bp 180°, Bp_{14} 73-75°.
Kannengiesser, G. *et al*, *Bull. Soc. Chim. Fr.*, 1967, 2492 (*synth*)
Buerger, H. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 2341.

Pacl, Z. *et al, Collect. Czech. Chem. Commun.*, 1971, **36**, 1588.
Gibbins, S.G. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 72 (*struct*)
Radeglia, R., *Z. Phys. Chem. (Leipzig)*, 1975, **256**, 453 (*nmr*)

IC-006312

$C_8H_{24}N_4Sn$

Tetrakis(dimethylamino)stannane, 8CI

Octamethylstannanetetramine, 9CI. Tetrakis(dimethylamino) tin

[1066-77-9]

$Sn(NMe_2)_4$

M 295.0
Liq. d_4^{20} 1.169. $Bp_{0.1}$ 53-55°.

Jones, K. *et al, J. Chem. Soc.*, 1965, 1944 (*synth*)
Buerger, H. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 2341 (*ir, raman*)
Vilkov, L.V. *et al, Zh. Strukt. Khim.*, 1970, **11**, 129; *CA*, **72**, 126014 (*struct*)
Harrison, P.G. *et al, J. Organomet. Chem.*, 1973, **55**, 261 (*mössbauer*)
Van den Berghe, E.V. *et al, J. Organomet. Chem.*, 1973, **61**, 197 (*nmr*)

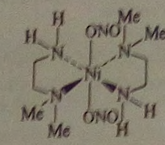
IC-006313

$C_8H_{24}N_6NiO_4$

Bis(*N,N*-dimethylethylenediamine)dinitritonickel(*II*)

Bis(N,N-dimethyl-1,2-ethanediamine-N,N')bis(nitrito-O) nickel, 11CI

[58893-98-4]



M 327.0
trans-Pseudooctahedral. Blue cryst. ($MeNO_2$). Sol. $MeNO_2$, $CHCl_3$, MeOH. Mp 212°. μ_{eff} = 3.25μ_B.

Goodgame, D.M.L. *et al, J. Chem. Soc.*, 1963, 5909 (*synth, uv-vis, magnetism*)
Goodgame, D.M.L. *et al, Inorg. Chem.*, 1964, **3**, 1389 (*uv-vis*)
Drew, M.G.B. *et al, Proc. Chem. Soc., London*, 1964, 363 (*cryst struct*)

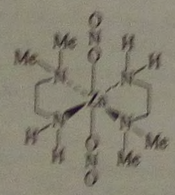
$C_8H_{24}N_4O_4Zn$

IC-006314

Bis(*N,N*-dimethylethylenediamine)dinitritozinc(*II*)

Bis(N,N-dimethyl-1,2-ethanediamine-N,N')bis(nitrito-O) zinc(II)

[80582-59-8]



M 333.7
trans-Octahedral molecule. Cryst. ($EtOH/Et_2O$).

[59855-69-0, 59926-77-7]

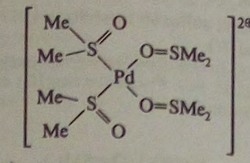
Goodgame, D.M.L. *et al, J. Chem. Soc. A*, 1970, 1333 (*synth, ir*)
Finney, A.J. *et al, Aust. J. Chem.*, 1981, **34**, 2061 (*cryst struct*)

$C_8H_{24}O_4PdS_4^{2\oplus}$

IC-006315

Tetrakis(dimethyl sulfoxide)palladium(*II*)(2+)

Tetrakis(methyl sulfoxide)palladium(II)(2+), 8CI. Bis[sulfinylbis[methane]-O]bis[sulfinylbis[methane]-S] palladium(II)(2+), 9CI



M 418.9 (ion)
cis-Square planar struct. Only one form known. Bulkier R_2SO favour *O*-binding. Synth. from Palladium(*II*) chloride ($PdCl_2$), IC-016770 or $[Pd(MeCN)_4]^{2\oplus}$ + DMSO.

Bis-tetrafluoroborate: [30079-58-4].
Yellow platelets (DMSO). Sol. DMSO.

[77648-62-5]

Wayland, B.B. *et al, Inorg. Chem.*, 1969, **8**, 971 (*synth, ir*)
Price, J.H. *et al, J. Chem. Soc., Chem. Commun.*, 1970, 1377 (*ir*)
Johnson, B.F.G. *et al, Acta Crystallogr., Sect. B*, 1981, **37**, 953 (*cryst struct*)

$C_8H_{24}O_4S_4Zn^{2\oplus}$

IC-006316

Tetrakis(dimethyl sulfoxide)zinc(2+)

Tetrakis[sulfinylbis[methane]-O]zinc(2+), 9CI

$[Zn(O{=}SMe_2)_4]^{2\oplus}$

M 377.9 (ion)
Dichloride: [31224-21-2]. *Zinc(II) chloride tetrakis(dimethyl sulfoxide)*
White cryst.
Bis-tetrafluoroborate: [19973-67-2].
White cryst.
Diperchlorate: [108558-33-4].
White cryst. (Me_2CO). Mp 73-74°.
▷ Potentially explosive.

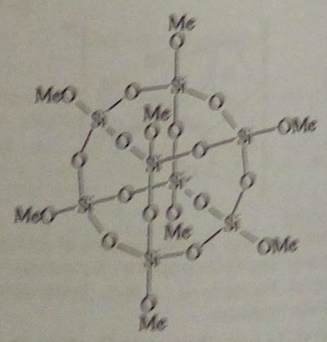
Selbin, J. *et al, J. Inorg. Nucl. Chem.*, 1961, **16**, 219 (*synth, ir, perchlorate*)
Kůtek, F., *Collect. Czech. Chem. Commun.*, 1968, **33**, 1930 (*synth, ir, tetrafluoroborate*)
Sljukic, M. *et al, Z. Kristallogr., Kristallogeom., Kristallphys., Kristallchem.*, 1970, **132**, 240 (*synth, cryst struct, chloride*)

$C_8H_{24}O_{20}Si_8$

IC-006317

Octamethoxypentacyclo[9.5.1.1^{3,9}.1^{5,15}.1^{7,13}]octasiloxane, 11CI

[98922-99-7]



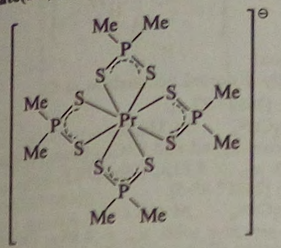
M 664.9
Each Si atom is located at corner of a cube with doubly bridging O atoms linking the Si centres along the cube edges. Terminal OMe groups at each Si. Colourless cryst. Sol. MeCN, toluene. Sublimes.

Day, V.W. *et al, J. Am. Chem. Soc.*, 1985, **107**, 8262 (*synth, Si-29 nmr*)

IC-006318

$C_8H_{24}P_4PrS_8^{\ominus}$

Tetrakis(dimethylphosphinodithioato-*S,S'*) praseodymate(*III*)(1−)



M 641.6 (ion)
8-Coord. distorted tetragonal antiprismatic struct. Similar compds. obt. for other lanthanides.

Ph_4P salt: [62389-66-6].
Pale green needles (EtOH). Sol. hot EtOH.
Ph_4As salt: [83729-94-6].
Green solid. Sol. CH_2Cl_2.

Pinkerton, A.A. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 2464; 1978, 85 (*synth, cryst struct, Ph_4P salt*)
Spiliadis, S. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 1815 (*synth, pmr, P-31 nmr*)

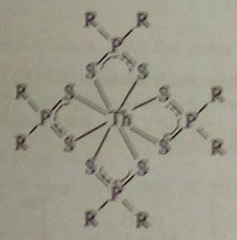
$C_8H_{24}P_4S_8Th$

IC-006319

Tetrakis(dimethylphosphinodithioato-*S,S'*)thorium(*IV*), 10CI

Tetrakis(dimethyldithiophosphinato)thorium(IV)

[79152-26-4]



R = Me

M 732.7
Dodecahedral. White cryst. Sol. CH_2Cl_2.

Pinkerton, A.A. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1475 (*synth, cryst struct, pmr, ir*)

$C_8H_{24}P_4S_8Tm^{\ominus}$

IC-006320

Tetrakis(dimethylphosphinodithioato-*S,S'*)thulate(*III*)(1−)

Tetrakis(dimethyldithiophosphinato)thulate(III)(1−)

$[Tm(S_2PMe_2)_4]^{\ominus}$

M 669.6 (ion)
8-Coord.

Ph_4P salt: [66484-24-0].
Cryst. Sol. EtOH, $CHCl_3$.
Ph_4As salt: [83729-95-7].
V. moisture-senstive cryst. Sol. CH_2Cl_2.

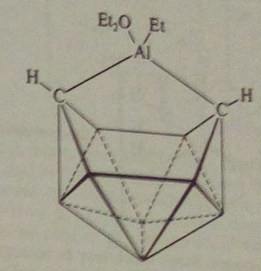
Pinkerton, A.A. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 85 (*synth, ir*)
Spiliadis, S. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 1809, 1815 (*pmr, P-31 nmr, cryst struct*)

$C_8H_{25}AlB_9O$

IC-006321

(6,9-Dicarbadecaborane(12)-6,9-diyl)(diethyl ether) ethylaluminium

[105581-63-3]



M 250.7
nido-. Colourless viscous air- and moisture-sensitive liq. Sol. toluene, spar. sol. pentane. $Bp_{0.001}$ 60°. Ir ν_{B-H} 2548 cm^{-1}. THF-d_8 analogue also known.

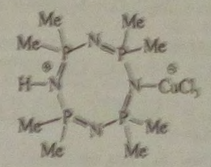
C_6H_6 solvate: [105581-65-5].
Cryst. Mp 28-30°.

Schubert, D.M. *et al, Organometallics*, 1987, **6**, 201 (*synth, cryst struct, pmr, B-11 nmr, ir*)

$C_8H_{25}Cl_3CuN_4P_4$

IC-006322

Trichloro(octamethylcyclotetraphosphonitrilium) copper(*II*)



M 471.1
Obt. by recryst. of octamethylcyclotetraphosphonitrile with $CuCl_2$ in 2-butanone. Yellow needles.

Trotter, J. *et al, J. Chem. Soc. A*, 1970, 455 (*synth, cryst struct*)

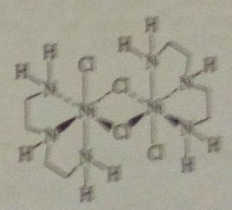
$C_8H_{28}Cl_4N_6Ni_2$

IC-006323

Tetrachlorobis(diethylenetriamine)dinickel(*II*)

Bis[N-(2-aminoethyl)-1,2-ethanediamine-N,N',N'']di-μ-chlorodichlorodinickel, 9CI

[22470-21-9]

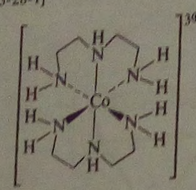


M 465.5
Proposed struct. shown, distorted octahedral coordination around Ni. Synth. from $NiCl_2.6H_2O$ and triethylenediamine followed by dehydration of hydrates over P_2O_5 or recryst. from EtOH. Hard, clear, green cryst., non-bridging Cls may be substituted by H_2O on exp. to atmospheric moisture. $\mu_{eff} = 3.01\mu_B$ (292K).

Breckenridge, J.G., *Can. J. Res., Sect. B*, 1948, **26**, 11 (*synth*)
Curtis, N.F. *et al*, *J. Chem. Soc. A*, 1968, 3069 (*uv, ir, props*)

IC-006324

$C_8H_{26}CoN_6^{3\oplus}$
Bis(diethylenetriamine)cobalt(*III*)(3+)
Bis[N-(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″]*cobalt*(3+), *9Cl*
[18703-28-1]



fac-sym-form

M 265.2 (ion)
Exists in 3 isomeric forms which may be separated chromatographically or by fractional crystallistion.

fac-symm-form [38318-04-6]
s-fac-*form*
Tribromide: [28993-35-3].
Red-orange prisms. Co—N_{sec} 195, Co—N_{term} 197 pm.

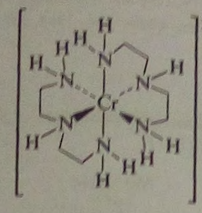
fac-asymm-form [38318-05-7]
u-fac-*form*
Hexakis(*cyano*-C)*cobaltate*(3−): Orange-red cryst. + $2H_2O$. Co—N 196-197 pm.

mer-form [38318-06-8]
Has been resolved.
Tribromide: [72597-11-6].
Yellow cryst. + $2H_2O$. Co—N_{sec} 194.0, CoN_{term} 198.1 pm.
Trinitrate: [58957-78-1].
Yellow cryst. + H_2O (H_2O). Co—N_{sec} 194.6; Co—N_{term} 197 pm.

[28993-34-2, 29116-22-1, 29636-13-3, 35195-06-3, 35195-09-6, 35195-10-9, 48145-49-9]

Mann, F.G., *J. Chem. Soc.*, 1934, 466 (*synth*)
Kobayashi, M. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 470 (*cryst struct*)
Yoshikawa, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 179 (*synth, isomers, ir, uv-vis, pmr, cd, chromtog, abs config*)
Keene, F.R. *et al*, *Inorg. Chem.*, 1972, **11**, 148 (*synth, resoln, ord, ir, pmr*)
Konno, M. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 739 (*cryst struct, abs config, u-fac-form*)
Inorg. Synth., 1973, **14**, 58 (*synth, uv-vis*)
Yoshikawa, Y., *Bull. Chem. Soc. Jpn.*, 1976, **49**, 159 (*isom*)
Sanalio, F.D. *et al*, *Inorg. Chem.*, 1976, **15**, 1626 (*cryst struct, pmr, cmr, mer-form*)
Searle, G.H. *et al*, *Aust. J. Chem.*, 1977, **30**, 1221 (*pmr, cmr*)
Okayama, K. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2389 (*cryst struct, mer-form, abs config*)

$C_8H_{26}CrN_6^{2\oplus}$
Bis(diethylenetriamine)chromium(*II*)(2+), 8Cl IC-006325
Bis[N-(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″]*chromium*(2+), *11Cl, 10Cl, 9Cl*

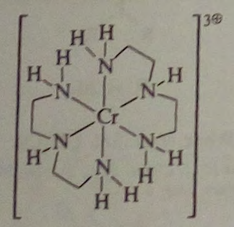


M 258.3 (ion)
Tetragonally distorted octahedron at Cr.
Dichloride: [24887-87-4].
$C_8H_{26}Cl_2CrN_6$ M 329.2
Synth. from ligand and $CrCl_2$. Blue, air-sensitive solid + $1H_2O$. $\mu_{eff} = 4.81\mu_B$ (90-300K).
Dibromide: [24887-88-5].
$C_8H_{26}Br_2CrN_6$ M 418.1
Blue air-sensitive solid. $\mu_{eff} = 4.88\mu_B$ (300K).
Diiodide: [24887-89-6].
$C_8H_{26}CrI_2N_6$ M 512.1
Blue air-sensitive solid. $\mu_{eff} = 4.84\mu_B$ (90-300K).
Diperchlorate: [71723-92-7].
Obt. by electrochem. redn. of corresp. Cr(*III*) complex. Known in soln. only.
▷ Isolation of solid could be hazardous.
Dicyclopentadienide: [105017-21-8].
$C_{18}H_{36}CrN_6$ M 388.5
Obt. by reaction of chromocene with diethylenetriamine. Air-sensitive grey powder. Sol. H_2O, EtOH with dec. $\mu_{eff} = 4.69\mu_B$ (r.t.).

[24917-12-2]

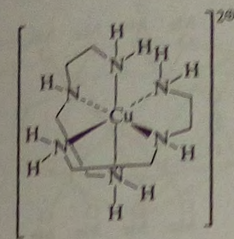
Earnshaw, A. *et al*, *J. Chem. Soc. A*, 1969, 2276 (*synth, props*)
Prügel, M. *et al*, *Z. Chem.*, 1976, **16**, 113 (*electrochem*)
Crouse, K. *et al*, *Inorg. Chim. Acta*, 1985, **99**, 199.
Kalousova, J. *et al*, *Collect. Czech. Chem. Commun.*, 1986, **51**, 314.
Micskei, K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 2721 (*stability const*)

$C_8H_{26}CrN_6^{3\oplus}$ IC-006326
Bis(diethylenetriamine)chromium(*III*)(3+)
Bis[N-(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″]*chromium*(3+), *11Cl, 10Cl, 9Cl*. *Bis*(*1,5-diamino-3-azapentane*)*chromium*(III)
[59691-88-2]



M 258.3 (ion)
Octahedral complex cation, no resolutions or structural assignments made.
Triperchlorate: [59691-89-3].
Hein, F. *et al*, *Ber.*, 1957, **90**, 928.
Kling, O. *et al*, *Z. Anorg. Allg. Chem.*, 1961, **313**, 187 (*synth, uv*)
Garner, C.S. *et al*, *Transition Met. Chem.*, 1970, **6**, 59 (*rev*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 806 (*rev*)

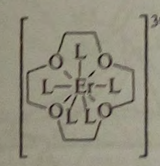
$C_8H_{28}CuN_6^{2\oplus}$ IC-006327
Bis(diethylenetriamine)copper(2+), 9Cl
Bis[N-(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″]*copper*(2+)
[34314-13-1]



M 269.8 (ion)
Approx. *mer*-octahedral cation.
Dibromide: [25778-27-2].
Dark blue plates + $1H_2O$.
Dinitrate: [27383-08-0].
Royal blue needles.

Hathaway, B.J. *et al*, *J. Chem. Soc. A*, 1969, 2312 (*uv-vis, esr, synth*)
Stephens, F.S., *J. Chem. Soc. A*, 1969, 883, 2233 (*cryst struct*)
Morpurgo, L. *et al*, *Biochim. Biophys. Acta*, 1973, **322**, 204 (*uv-vis, esr, reactions*)

$C_8H_{26}ErO_9^{3\oplus}$ IC-006328
Pentaaqua(12-crown-4)erbium(*III*)(3+)
Erbium(3+) (*12-crown-4*) *pentahydrate*. *Pentaaqua*(*1,4,7,10-tetraoxacyclododecane*-O^1,O^4,O^7,O^{11})*erbium*(3+)

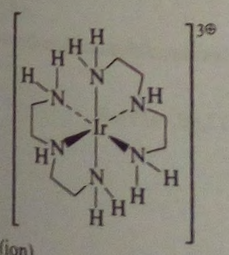


L = OH_2

M 433.5 (ion)
9-Coord. Similar compds. obtd. for other lanthanides: Ce, Nd, Sm, Eu, Gd, Tb, Dy, Ho.
Trichloride: [116747-29-6].
$C_8H_{26}Cl_3ErO_9$ M 539.9
Pink cryst. + $2H_2O$ (MeCN/MeOH). Sol. MeCN. Dehydrates at *ca.* 68-75°.

Rogers, R.D. *et al*, *Inorg. Chem.*, 1988, **27**, 3826 (*synth, cryst struct*)

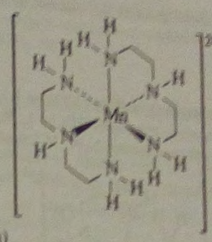
$C_8H_{24}IrN_6^{3\oplus}$ IC-006329
Bis(diethylenetriamine)iridium(*III*)(3+)
Bis[N-(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″]*iridium*(3+)



fac-form

M 398.5 (ion)

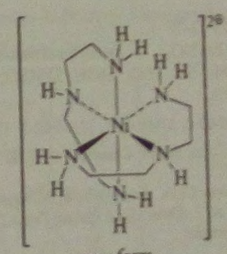
$C_8H_{26}MnN_6^{2\oplus}$
Bis(diethylenetriamine)manganese(*II*)(2+) IC-006330
Bis[N-(*2-aminoethyl*)-*1,2-ethanediamine*-N,N′,N″]*manganese*(II)(2+), *10Cl*



M 261.2 (ion)
Octahedral. Synth. from $MnCl_2.4H_2O$, excess dien $N_2H_4.H_2O$ in H_2O. Catalyst for the dec. of H_2O_2. Accelerates photopolymerisation of vinyl monomers in the presence of CCl_4. Air-sensitive in soln. Reacts with bipy in aq. soln. to give $[Mn(dien)bipy]^{2\oplus}$.
Dibromide:
$C_8H_{26}Br_2MnN_6$ M 421.0
Synth. by adding $MnBr_2.H_2O$ to dien at 0° under He. Air-sensitive white cryst. Insol. MeOH, EtOH, MeCN, dioxan, γ-butyrolactone. Sol. DMSO. Mp 210-265° dec. High spin manganese(*II*) complex. $\mu_{eff} = 6.1\mu_B$ (298K). Reacts with liquid NH_3 at −35° to give $[Mn(NH_3)_6]Br_2$.
Diperchlorate:
$C_8H_{26}Cl_2MnN_6O_8$ M 460.1
Synth. by adding aq. 5*M* $NaClO_4$ to $MnCl_2.4H_2O$, dien and $N_2H_4.H_2O$ in H_2O. White cryst.
▷ Potentially explosive.

Jonassen, H.B. *et al*, *J. Phys. Chem.*, 1952, **56**, 16 (*formation constants*)
Manhas, B.S., *Diss. Abstr.*, 1965, **26**, 685 (*ir, props*)
Langenbeck, W. *et al*, *J. Prakt. Chem.*, 1965, **27**, 64 (*props*)
Watt, G.W. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1945 (*magnetism, props*)
Joørgensen, C.K. *et al*, *Inorg. Chim. Acta*, 1969, **3**, 313 (*uv, props*)
Okimoto, T. *et al*, *Angew. Makromol. Chem.*, 1974, **38**, 81 (*props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, D3, 54 (*rev, bibl*)

$C_8H_{26}N_6Ni^{2\oplus}$ IC-006331
Bis(diethylenetriamine)nickel(*II*)(2+), 8Cl
Bis[N-(*2-aminoethyl*)-*1,2-ethanediamine*]*nickel*(II)(2+), *9Cl*. *Bis*[*bis*(*2-aminoethyl*)*amine*]*nickel*(II)(2+)



mer-form

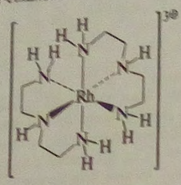
M 265.0 (ion)
Many salts known. Classic tridentate ligand.
mer-form [19358-75-9]
Dichloride, monohydrate: [15977-16-9].

$C_9H_{28}Cl_2N_4NiO$ M 353.9
Violet diamond-shaped plates. Sol. H_2O.
Trithiocarbonate(2−) salt: [38857-57-7].
Rose coloured solid.

[38594-21-5]
Curtis, N.F. *et al, J. Chem. Soc. A*, 1968, 3069 (*synth, uv*)
Biagini, S. *et al, J. Chem. Soc. A*, 1970, 2398 (*cryst struct*)
Fereday, R.J. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 197 (*uv-vis*)
Roger, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1973, **277**, 1231 (*deriv*)

IC-006332

$C_9H_{20}N_6Rh^{3\oplus}$
Bis(diethylenetriamine)rhodium(*III*)(3+)
*Bis[1,4,7-triazaheptane)rhodium(*III*)(3+). Bis[N-(2-aminoethyl)-1,2-ethanediamine-N,N′,N″]rhodium(3+)*

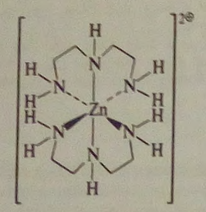


M 309.2 (ion)
Prob. struct. shown.
Trichloride: [52033-06-4].
$C_9H_{28}Cl_3N_6Rh$ M 415.5
Cryst.
Triiodide: [14242-45-6].
Colourless cryst. +1H_2O (H_2O). Sol. H_2O. Diamagnetic.

Schmidtke, H.-H., *Z. Phys. Chem. (Frankfurt am Main)*, 1963, **38**, 170 (*synth, uv-vis*)
Watt, G.W., *Inorg. Chem.*, 1965, **4**, 143 (*synth, ir*)

IC-006333

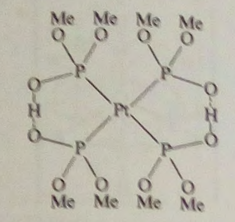
$C_9H_{20}N_6Zn^{2\oplus}$
Bis(diethylenetriamine)zinc(2+)
Bis[N-(2-aminoethyl)-1,2-ethanediamine-N,N′,N″]zinc(2+)
[46358-79-6]



M 271.7 (ion)
Dinitrate: [36913-52-7].
Prepd. from $Zn(NO_3)_2$ + diethylenetriamine in EtOH. Cryst. (MeOH). Sol. H_2O, EtOH, DMSO; insol. MeOH, Me_2CO, $CHCl_3$.

[22470-18-4, 37566-00-0, 37566-01-1, 37566-02-2, 37566-03-3]
Zocchi, M. *et al, Cryst. Struct. Commun.*, 1972, **1**, 135 (*cryst struct, nitrate*)
Cova, G. *et al, Inorg. Chim. Acta*, 1972, **6**, 343 (*synth, ir*)
Hodgson, P.G. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1870 (*cryst struct, bromide*)

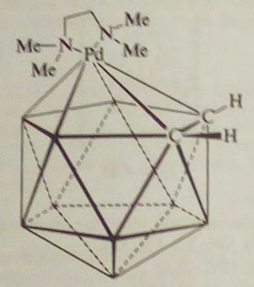
$C_9H_{20}O_{12}P_4Pt$ **IC-006334**
Bis(dimethylphosphonic acid)bis(dimethylphosphonito)platinum(*II*)
Tetrakis(dimethylphosphito)platinum(2−)dihydrogen, 10Cl
[30053-63-5]



M 633.2
Example of secondary phosphite complex. Synth. from $Pt[P(OMe)_3]_4^{2\oplus}$ + $4OH^{\ominus}$. White cryst. Mp 110° dec. Et analogue also known.

Sperline, R.P. *et al, Inorg. Chem.*, 1978, **17**, 2032 (*pmr*)
Solar, J.M. *et al, Inorg. Chem.*, 1984, **23**, 373, 758 (*synth, P-31 nmr, uv, cryst struct*)

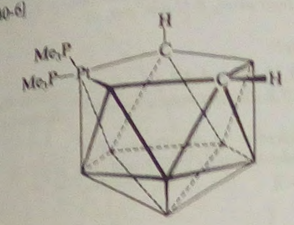
$C_9H_{27}B_9N_2Pd$ **IC-006335**
[(7,8,9,10,11-η)-7,8-Dicarbaundecaborato(2−)-][(*N,N,N′,N′*-tetramethylethanediamine-*N,N′*)palladium, 10Cl
3-(N,N,N′,N′-Tetramethylethanediamine)-1,2-dicarba-3-palladadodecaborane
[67538-15-2]



M 355.0
closo-. Dark-green cryst. (CH_2Cl_2/pentane). Sol. CH_2Cl_2. Mp >300°.

Colquhoun, H.M. *et al, J. Chem. Soc., Chem. Commun.*, 1978, 322 (*cryst struct*)
Colquhoun, H.M. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 761 (*synth, cryst struct, B-11 nmr, pmr, ir*)

$C_9H_{28}B_9P_2Pt$ **IC-006336**
[η⁵-Decahydrodicarbadecaborato(2−)][bis(trimethylphosphine)platinum, 9Cl
[58348-40-6]

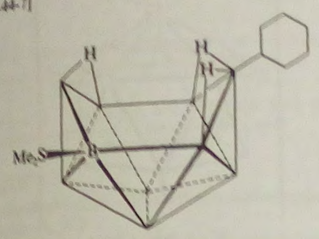


M 467.8
nido-. Pale-yellow cryst. (CH_2Cl_2). Sol. CH_2Cl_2. Mp 283°.

Barker, G.K. *et al, J. Chem. Soc., Chem. Commun.*, 1975, 804 (*synth, cryst struct*)

IC-006337

$C_9H_{19}B_{10}S$
9-Cyclohexyl-5-(dimethyl sulfide)decaborane(11)
[72765-44-7]



M 264.4
nido-. Colourless cryst. (C_6H_6/cyclohexane). Sol. C_6H_6, toluene, cyclohexane, EtOAc. Mp 75-76°.

Tolpin, E.I. *et al, Inorg. Chem.*, 1980, **19**, 1182 (*synth, uv, ir, pmr, B-11 nmr, cmr*)
Mizusawa, E. *et al, Inorg. Chem.*, 1980, **19**, 1188 (*cryst struct*)

$C_9H_{28}Br_2MnN_4$ **IC-006338**
Dibromotetrakis(ethylamine)manganese(*II*)
Manganese(II) bromide tetrakis(ethylamine)

$MnBr_2(NH_2Et)_4$

M 395.0
Synth. by passing $EtNH_2$ over anhydrous $MnBr_2$ at r.t. Chloride and iodide derivs. also known.

Ephraim, F. *et al, Ber. Dtsch. Chem. Ges.*, 1913, **46**, 3742 (*synth, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 21 (*rev, bibl*)

$C_9H_{28}Cl_2P_4Ru$ **IC-006339**
Dichlorotetrakis(dimethylphosphine)ruthenium(*II*), 9Cl
[58341-36-9]

$Ru(PMe_2H)_4Cl_2$

M 420.1
Only *trans* isomer known; Ru—Cl 244, Ru—P 232.7 pm. Prepd. by treating $RuCl_3.xH_2O$ with P_2Me_4 in boiling EtOH. Yellow cryst. Sol. C_6H_6. Mp 209-210°. Subl. 145-175° *in vacuo*.

Cotton, F.A. *et al, Inorg. Chim. Acta*, 1976, **16**, 203 (*synth, cryst struct, ir, pmr, ms*)

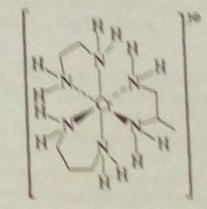
$C_9H_{28}Cl_4Mo_2N_4$ **IC-006340**
Tetrachlorotetrakis(dimethylamine)dimolybdenum(*II*)
Tetrachlorotetrakis(N-methylmethanamine) dimolybdenum(II), 10Cl
[65863-82-3]

$(Me_2NH)_2Cl_2Mo{\equiv}MoCl_2(NHMe_2)_2$

M 514.0
Synth. by treatment of $MoCl_3$ with Me_2NH. Purple powder. Insol. most org. solvs. Diamagnetic.

Edwards, D.A. *et al, Inorg. Chim. Acta*, 1977, **25**, L47 (*synth, ir, reflectance, magnetism*)
Armstrong, J.E. *et al, Inorg. Chem.*, 1979, **18**, 1172 (*synth, ir, reflectance, magnetism, pe*)

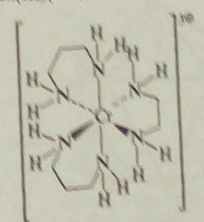
$C_9H_{28}CrN_6^{3\oplus}$ **IC-006341**
(1,2-Ethanediamine-*N,N′*)(1,2-propanediamine-*N,N′*)(1,3-propanediamine-*N,N′*)chromium(*III*)(3+), 1ICl
(Ethylenediamine)(propylenediamine)(trimethylenediamine) chromium(III)



M 260.3 (ion)
Mixed diamine octahedral complex.
Trichloride: [81194-15-2].
Yellow cryst. +2H_2O (H_2O). Loses H_2O at 80-160°. Loses some ethylenediamine at 200-225°.
Trithiocyanate: [81194-14-1].
Obt. by metathesis of chloride with $(NH_4)SCN$. Loses some ethylenediamine at 120-160°.

Uehara, A. *et al, Inorg. Chem.*, 1982, **21**, 2422 (*synth, thermal dec*)

$C_9H_{28}CrN_6^{3\oplus}$ **IC-006342**
(Ethylenediamine)bis(1,3-propanediamine)chromium(*III*)(3+)
(1,2-Ethanediamine-N,N′)bis(1,3-propanediamine-N,N′) chromium(III)(3+), 1ICl, 10Cl.9Cl



A-form

M 260.3 (ion)
A-form

(+)-form

Tribromide: [39023-35-3].
Obt. by mixing racemic chloride in aq. soln. with $(+)_D$ sodium salt of α-nitro-$(+)_D$-camphor, then adding HBr. Solid.

(±)-form [78404-07-6]

Trichloride: [41101-31-9].
Yellow cryst. + H_2O (H_2O). Dehydrates at 100-160°; deaminates at 190-230°.

Triiodide: [77370-99-1].
Yellow cryst. + $2H_2O$.

Trithiocyanate: [81194-20-9].
Cryst. + $0.5H_2O$. Dehydrates at 70-90°, deaminates at 100-150°.

[68193-89-5]

Rancke-Madsen, M. *et al, Acta Chem. Scand.*, 1972, **26**, 3405 (*optical activity*)
Duesler, E.N. *et al, Inorg. Chim. Acta*, 1978, **30**, 87 (*cryst struct, iodide*)
Jensen, H.P., *Acta Chem. Scand., Ser. A*, 1981, **35**, 127 (*optical activity, cd*)
McLean, J.A. *et al, Inorg. Chim. Acta*, 1981, **53**, L43 (*synth, uv-vis*)
Uehara, A. *et al, Inorg. Chem.*, 1982, **21**, 2422 (*synth, thermal dec*)

$C_8H_{28}N_4Pt^{2\oplus}$ IC-006343

Tetrakis(ethylamine)platinum(*II*)(2+), 8Cl

Tetrakis(ethanamine)platinum(2+), 9Cl

[21430-92-2]

$[Pt(NH_2Et)_4]^{2\oplus}$

M 375.4 (ion)
There is special interest in salts of $[PtX_4]^{2\ominus}$, green colour indicating stacked struct.with weak Pt—Pt interactions. Salts of $[PdX_4]^{2\ominus}$ also known.

Tetrachloroplatinate(2−): [14242-49-0].
$C_8H_{28}Cl_4N_4Pt_2$ M 712.3
Pink needles, colourless in soln. Sol. H_2O.

Tetrabromoplatinate(2−): [14242-46-7].
$C_8H_{28}Br_4N_4Pt_2$ M 890.1
Green solid, red in soln. Sol. H_2O.

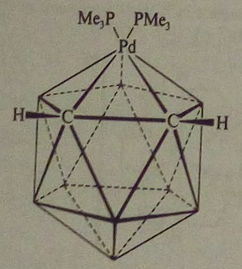
Miller, J.R., *J. Chem. Soc.*, 1961, 4452; 1965, 713 (*uv-vis*)
Anex, B.G. *et al, J. Chem. Phys.*, 1967, **46**, 1090 (*uv-vis*)
Cradwick, E.M. *et al, Acta Crystallogr., Sect. B*, 1971, **27**, 480 (*cryst struct*)

$C_8H_{29}B_9P_2Pd$ IC-006344

[(7,8,9,10,11-η)-7,8-Dicarbaundecaborato(2−)] bis(trimethylphosphine)palladium, 10Cl

3,3-Bis(trimethylphosphine)-1,2-dicarba-3-palladadodecaborane

[67538-14-1]



M 390.9

closo-. Dark-red cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2. Mp 149°.

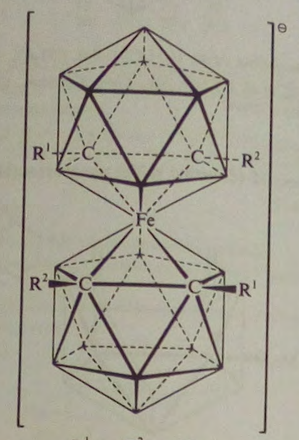
Colquhoun, H.M. *et al, J. Chem. Soc., Chem. Commun.*, 1978, 322 (*cryst struct*)
Colquhoun, H.M. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 761 (*synth, cryst struct, B-11 nmr, pmr, ir*)

$C_8H_{30}B_{18}Fe^{\ominus}$ IC-006345

Bis[(7,8,9,10,11-η)-1,2,3,4,5,6,9,10,11-nonahydro-7,8-dimethyl-7,8-dicarbaundecaborato(2−)]ferrate(1−), 10Cl

Bis[undecahydro-7,8-dimethyl-π-7,8-dicarbaundecaborato(2−)]ferrate(1−), 8Cl

[11070-28-3]



$R^1 = R^2 = Me$

M 376.7 (ion)
Paramagnetic. Reduced to a deep-lavender-blue ferrate (2−) species.

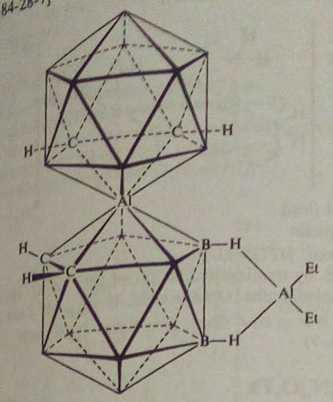
Me_4N salt: [12556-51-3].
Red cryst. (Me_2CO aq.). Mp 247-249°.

Gray, H.B. *et al, Inorg. Chem.*, 1971, **10**, 1559 (*magnetism*)
Ammeter, J.H. *et al, J. Magn. Reson.*, 1978, **30**, 299 (*esr*)

$C_8H_{32}Al_2B_{18}$ IC-006346

Diethyl[μ-[(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)-*H*²:*H*′]][(7,8,9,10,11-η)-undecahydro-7,8-dicarbaundecaborato(2−)]dialuminium

[103384-28-7]



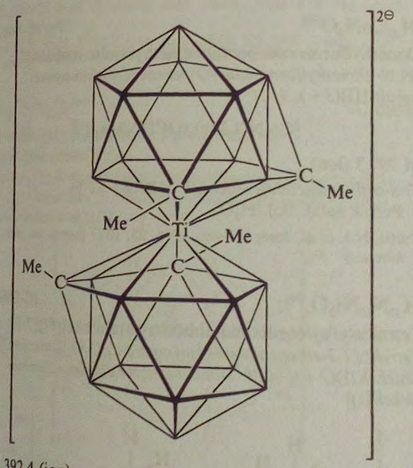
M 376.9
Formed by Co-catalysed dimerisation of 3-Ethyl-3-aluminio-1,2-dicarba-*closo*-dodecaborane(12), IC-004312.

Rees, W.S. *et al, J. Am. Chem. Soc.*, 1986, **108**, 5367; 1987, **109**, 2861 (*synth, cryst struct, ir, pmr, cmr, B-11 nmr*)

$C_8H_{32}B_{20}Ti^{2\ominus}$ IC-006347

Bis[η⁵-decahydro-*C,C′*-dimethyldicarbadodecaborato(2−)]titanate(2−), 9Cl

4,4′-Bis(decahydro-1,6-dimethyl-1,6-dicarba-4-titana-closo-tridecaborate)(2−)



M 392.4 (ion)

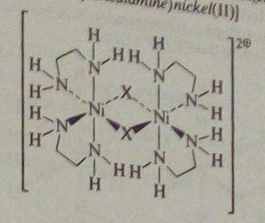
Bis-Me_4N salt: [55266-92-7].
Red cryst. + $2Me_2CO$ (Me_2CO/EtOH), air-stable in solid state.

Salentine, C.G. *et al, J. Am. Chem. Soc.*, 1975, **97**, 426 (*synth, pmr, nmr, props*)
Yo, F.Y. *et al, J. Am. Chem. Soc.*, 1975, **97**, 428 (*cryst struct*)

$C_8H_{32}Br_2N_8Ni_2^{2\oplus}$ IC-006348

Di-μ-bromotetrakis(ethylenediamine)dinickel(*II*)(2+)

Di-μ-bromobis[bis(ethylenediamine)nickel(II)]



X = Br

M 517.5 (ion)
Magnetic susceptibilities indicate ferromagnetic intradimer exchange interaction.

Dibromide: [21479-61-8].
$C_8H_{32}Br_4N_8Ni_2$ M 677.3
Synth. from $NiBr_2.6H_2O$ and $[Ni(H_2NCH_2CH_2NH_2)_3]$ $Br_2.2H_2O$. $\mu_{eff} = 3.07\mu_B$ (292K).

Ginsberg, A.P. *et al, Inorg. Chem.*, 1972, **11**, 2884 (*synth, deriv*)
Lever, A.B.P. *et al, Can. J. Chem.*, 1973, **51**, 1567 (*ir, deriv*)
Stebler, A. *et al, Inorg. Chem.*, 1982, **21**, 380 (*magnetism*)

$C_8H_{32}Br_2N_8OZr$ IC-006349

Dibromotetrakis(1,1-dimethylhydrazine-*N*²)oxozirconium(*IV*), 11Cl

[81599-48-6]

$(Me_2NNH_2)_4ZrOBr_2$

M 507.4
Synth. from $ZrOBr_2$ and 1,1-dimethylhydrazine in ethanol. White, hygroscopic solid. Insol. EtOH, Et_2O. Analogues of hydrazine and phenylhydrazine also descr. See Dichlorooxotetrakis(phenylhydrazine-*N*²)zirconium(*IV*), IC-011459.

Srivastava, A.K. *et al, Transition Met. Chem.*, 1982, **7**, 41 (*synth, ir, dta*)

$C_8H_{32}Cl_2N_8Ni_2^{2\oplus}$ IC-006350

Di-μ-chlorotetrakis(ethylenediamine)dinickel(*II*)(2+)

Di-μ-chlorobis[bis(ethylenediamine)nickel(II)]

As Di-μ-bromotetrakis(ethylenediamine)dinickel(*II*)(2+), IC-006348 with

X = Cl

M 428.6 (ion)
Magnetic susceptibilities indicate ferromagnetic intradimer exchange interaction.

Dichloride: [20647-35-2].
$C_8H_{32}Cl_4N_8Ni_2$ M 499.5
Synth. from $[Ni(H_2NCH_2CH_2NH_2)_3]Cl_2.2H_2O$ and $NiCl_2.6H_2O$. Blue cryst. V. sol. H_2O, sol. MeOH, spar. sol. Me_2CO, EtOH. $\mu_{eff} = 3.15\mu_B$ (297K), dec. at 290°.

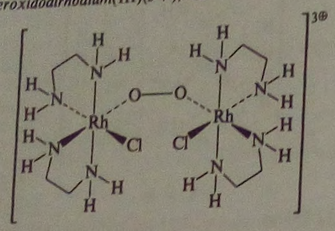
Diperchlorate: [15692-12-3].
Blue cryst.
▷ Potentially explosive.

Inorg. Synth., 1960, **6**, 198 (*synth, props, dichloride*)
Curtis, N.F. *et al, J. Chem. Soc. A*, 1968, 3069 (*synth, ir, uv, deriv*)
Ebner, J.R. *et al, Inorg. Chem.*, 1976, **15**, 3014 (*pe*)
Joung, K.O. *et al, Inorg. Chem.*, 1979, **18**, 804 (*cryst struct, dichloride*)

$C_8H_{32}Cl_2N_8O_2Rh_2^{3\oplus}$ IC-006351

Dichlorotetrakis(ethylenediamine) superoxidodirhodium(*III*)(3+)

Dichlorotetrakis(1,2-ethanediamine-N,N′)-μ-superoxidodirhodium(III)(3+), *11Cl*



M 549.1 (ion)

Prob. octahedral with bridging $O_2^{\ominus}$, but whether *cis* or *trans* isomer not detected.

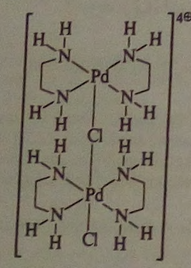
Trichloride: [82532-97-6].
Sol. H_2O.

Raynor, J.B. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 1165 (*synth, theory, esr*)

$C_8H_{32}Cl_2N_8Pd_2^{4\oplus}$ IC-006352

Dichlorotetrakis(ethylenediamine)dipalladium(*II,IV*)(4+)

μ-Chlorochlorotetrakis(1,2-ethanediamine-N,N′) dipalladium(4+), *9Cl*



M 524.1 (ion)

Uncertain whether bridging Pd—Cl distances are equal or whether struct. is a 1-dimensional polymer. Synth. from Bis(ethylenediamine)palladium(*II*)(2+), IC-004380 + HNO_3 or $HClO_4$.

Tetranitrate: [9076-08-8].
Dark green cryst. Sol. H_2O.

Tetraperchlorate: [9047-90-9].
Dark green needles. Sol. H_2O.

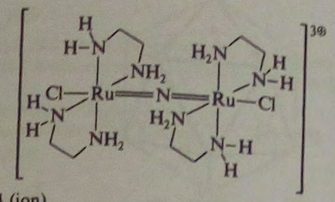
▷ Potentially explosive.

Mason, W.R., *Inorg. Chem.*, 1973, **12**, 20 (*synth, uv*)

$C_8H_{32}Cl_2N_9Ru_2^{3\oplus}$ IC-006353

Dichlorotetrakis(ethylenediamine)-μ-nitridodiruthenium(*IV*)(3+)

Dichlorotetrakis(1,2-ethanediamine-N,N′)-μ-nitridodiruthenium(3+). *μ-Nitridobis[chlorobis(1,2-diaminoethane)ruthenium*(IV)]



M 527.4 (ion)

Diamagnetic.

Trichloride: [42735-83-1].
Prepd. by treating $[Ru_2NCl_8(OH_2)_2]^{3\ominus}$ in aq. HCl with ethylenediamine. Orange solid. Ir ν_{Ru_2N} 1052 cm^{-1}.

Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)

$C_8H_{32}Cl_4N_{16}O_8Th$ IC-006354

Tetrachlorooctakis(urea)thorium(*IV*), 8Cl

Octakis(urea)thorium(4+) *tetrachloride. Thorium*(IV) *chloride octakis-urea*

[20539-67-7]

$$[Th(urea)_8]^{4\oplus}(Cl^{\ominus})_4$$

M 854.2

Probable ionic formulation shown. Hygroscopic colourless cryst. Sol. MeOH, EtOH, Me_2CO, H_2O. Similar iodide and bromide obt. Dec. > 135°.

Molodkin, A.K. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1967, **12**, 963; 1968, **13**, 1192; 1969, **14**, 215 (*synth, ir*)

$C_8H_{32}CoN_6O^{3\oplus}$ IC-006355

Dimethylformamidepentakis(methylamine)cobalt(*III*)

(*N,N-Dimethylformamide*-O)*pentakis(methanamine) cobalt*(III)(3+), *11Cl*

$$[Co(NH_2Me)_5(OCHNMe_2)]^{3\oplus}$$

M 287.3 (ion)

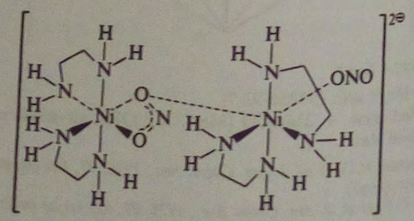
Tris-trifluoromethanesulfonate: [100681-52-5].
Purple solid. Sol. H_2O.

Curtis, N.J. *et al, Inorg. Chem.*, 1986, **25**, 1033 (*synth, uv, pmr, kinetics*)

$C_8H_{32}N_{10}Ni_2O_4^{2\ominus}$ IC-006356

Tetrakis(ethylenediamine)bis(nitrito)dinickel(*II*)(2+)

Tetrakis(1,2-ethanediamine)[μ-(nitrito-O:O,O′)](nitrito-O) dinickel(II)(2+), *10Cl. Dinitritobis[bis(ethylenediamine) nickel*(II)]



M 449.7 (ion)

Has monodentate and monatomic bridging bidentate NO_2 coordinating only through O. Antiferromagnetic.

Bis-tetraphenylborate: [80890-40-0].
Dark blue cryst.

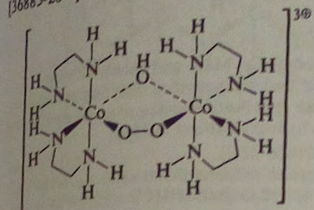
Gleizes, A. *et al, Inorg. Chem.*, 1982, **21**, 2257 (*synth, cryst struct, uv, magnetism*)

$C_8H_{33}Co_2N_8O_3^{3\oplus}$ IC-006357

Tetrakis(ethylenediamine)-μ-hydroxy-μ-peroxydicobalt(*III*)(3+)

Tetrakis(1,2-ethanediamine-N,N′)-μ-hydroxy[μ-(peroxy-O:O′)]dicobalt(III)(3+), *10Cl. μ-Hydroxo-μ-peroxobis[bis(ethylenediamine)cobalt*(III)]

[36885-26-4]



meso-form

M 407.2 (ion)

meso-form

The CoOOCo group is non planar. Distorted octahedral coord. at Co.

Triperchlorate: [58207-63-9].
Black cryst.
▷ Potentially explosive.

(±)-form

(ΔΛ, ΔΛ)-form

Dithionate, nitrate: [58692-02-7].
Brown cryst.

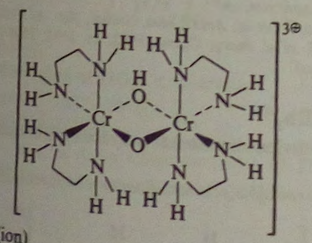
Thewalt, U. *et al, Z. Anorg. Allg. Chem.*, 1976, **419**, 163 (*synth, cryst struct*)

Fallab, S. *et al, Helv. Chim. Acta*, 1980, **63**, 1491 (*synth, cryst struct*)

$C_8H_{33}Cr_2N_8O_2^{3\oplus}$ IC-006358

Tetrakis(ethylenediamine)-μ-hydroxy-μ-oxodichromium(*III*)(3+)

μ-Oxo-μ-hydroxo-bis[bis(ethylenediamine)chromium(III)(3+)]. *Tetrakis(1,2-ethanediamine-N,N′)-μ-hydroxy-μ-oxodichromium*(III)(3+), *9Cl*



M 377.3 (ion)

Uncommon μ-oxo-μ-hydroxo dinuclear cation containing octahedral Cr. Blue aq. solns. rapidly dec. to reddish [(HO)(en)$_2$Cr(OH)Cr(en)$_2$(OH)] and then to Tetrakis(ethylenediamine)di-μ-hydroxydichromium(*III*)(4+), IC-006364 if acid added.

Triperchlorate: [57159-04-3].
Green cryst. Dec. in H_2O. Stable if dry.

Springborg, J. *et al, J. Chem. Soc., Chem. Commun.*, 1975, 422 (*synth, props*)

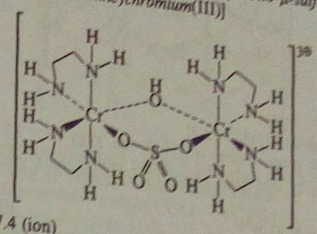
Springborg, J. *et al, Acta Chem. Scand., Ser. A*, 1976, **30**, 171 (*synth, props*)

Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 799 (*rev*)

$C_8H_{33}Cr_2N_8O_5S^{3\oplus}$ IC-006359

Tetrakis(ethylenediamine)-μ-hydroxy-μ-sulfatodichromium(*III*)(3+)

Tetrakis(1,2-ethanediamine-N,N′)-μ-hydroxy[μ-[sulfato(2−)-O:O′]]dichromium(III)(3+), *10Cl. μ-Hydroxo-μ-sulfato-bis[bis(ethylenediamine)chromium*(III)]



M 457.4 (ion)

Distorted octahedral Cr. Stable in acid and neutral soln.; deprotonates in base giving blue μ-oxo-μ-sulfato cation and then rapid sulfato-bridge cleavage.

Triperchlorate: [67369-33-9].
Synth. from Tetrakis(ethylenediamine)di-μ-hydroxydichromium(*III*)(4+), IC-006364 and 0.5*M* H_2SO_4. Red cryst. (0.5*M* HCl/satd. $NaClO_4$). Spar. sol. H_2O; sol. 1*M* HCl, H_2SO_4 or LiCl.
▷ Potentially explosive.

Chloride, tetrachlorozincate: [67392-72-7].
Synth. from corresp. perchlorate in 0.5*M* HCl/4*M* Li_2ZnCl_4.

Dithionate (2:3): [67576-89-0].
Red cryst. Spar. sol. H_2O.

[70116-67-5]

Springborg, J., *Acta Chem. Scand., Ser. A*, 1978, **32**, 231 (*synth, ir*)
Kaas, K., *Acta Crystallogr., Sect. B*, 1979, **35**, 596 (*cryst struct*)

$C_8H_{34}CoN_5O_4P^{3\oplus}$ IC-006360

Pentakis(methylamine)(trimethylphosphate)cobalt(*III*)(3+)

Pentakis(methanamine)(trimethylphosphate-O‴)cobalt(III)(3+), *11Cl*

$$[Co(NH_2Me)_5O{=}P(OMe)_3]^{3\oplus}$$

M 354.2 (ion)

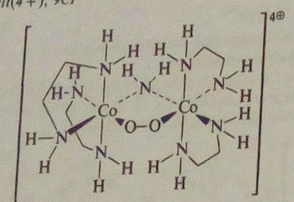
Tris-trifluoromethanesulfonate: [100681-45-6].
Purple solid. Sol. H_2O.

Curtis, N.J. *et al, Inorg. Chem.*, 1986, **25**, 1033 (*synth, uv, kinetics*)

$C_8H_{34}Co_2N_9O_2^{4\oplus}$ IC-006361

Amidotetrakis(ethylenediamine)superoxidodicobalt(*III*)(4+)

μ-Amidotetrakis(1,2-ethanediamine-N,N′)-μ-(superoxido)dicobalt(4+), 9CI



M 406.2 (ion)

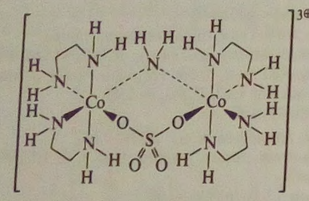
Tetranitrate: [16871-12-8].
Dark green needles + $1H_2O$. Sol. H_2O.

Thewalt, U. *et al, Inorg. Chem.*, 1972, **11**, 351 (*synth, cryst struct*)

$C_8H_{34}Co_2N_9O_4S^{3\oplus}$ IC-006362

μ-Amidotetrakis(1,2-ethanediamine-*N,N′*)[μ-(sulfato-*O:O′*)]dicobalt(*III*)(3+), 9CI

μ-Amido-μ-sulfatobis[bis(ethylenediamine)cobalt(III)](3+)



M 470.3 (ion)

Prepd. in soln. by reduction of $[(en)_2Co\text{-}\mu\text{-}(NH_2)\text{-}\mu\text{-}(O_2)Co(en)_2]^{3\oplus}$ by sulfite ions.

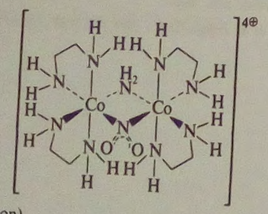
Tribromide: [24983-28-6].
No phys. props. reported. Sol. H_2O.

Stevenson, M.B. *et al, J. Chem. Soc. A*, 1969, 2979 (*synth, uv*)
Edwards, J.D. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1561 (*synth, uv, kinetics*)

$C_8H_{34}Co_2N_{10}O_2^{4\oplus}$ IC-006363

μ-Amidotetrakis(ethylenediamine-*N,N′*)[μ-(nitrito-*N:N*)]dicobalt(4+)

μ-Amido-μ-nitritobis[bis(ethylenediamine)cobalt(III)]. *μ-Amidotetrakis(1,2-ethanediamine-N,N′)[μ-(nitrito-N;N)]dicobalt(4+)*



M 420.2 (ion)

Prepd. by reduction of aq. $[(en)_2Co\text{-}\mu\text{-}NH_2\text{-}\mu\text{-}O_2\text{-}Co(en)_2]Br_4$. Not isol. as salts.

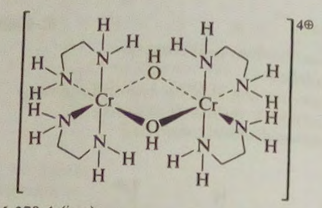
Edwards, J.D. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 1561 (*synth, uv, kinetics*)

$C_8H_{34}Cr_2N_8O_2^{4\oplus}$ IC-006364

Tetrakis(ethylenediamine)di-μ-hydroxydichromium(*III*)(4+), 8CI

Tetrakis(1,2-ethanediamine-N,N′)di-μ-hydroxydichromium(4+), 11CI, 10CI, 9CI. Di-μ-hydroxobis[bis(ethylenediamine)chromium(III)]

[47022-64-0]



meso-form

M 378.4 (ion)

Distorted octahedral Cr. Meso and racemic forms identified by ir and cryst. structs. Starting material for other dinuclear spp. Antiferromagnetic. In equilibrium with mono-μ-hydroxy cations in H_2O.

Tetrachloride: [71606-22-9].
Synth. from crude dithionate and satd. aq. NH_4Cl. Violet cryst. + $2H_2O$ (0.01*M* HCl/satd. NH_4Cl). Sol. H_2O.

Tetrabromide: [71606-23-0].
Synth. from crude dithionate in satd. aq. NH_4Br. Violet cryst. + $2H_2O$ (0.01*M* HBr/satd. NH_4Br). Mod. sol. H_2O.

Tetraiodide: [51456-45-2].

Diperchlorate, dichloride: [59366-53-9].
Blue-violet cryst.

Tetraperchlorate: [62661-31-8].
Synth. from crude bromide and satd. aq. $NaClO_4$. Violet cryst. (0.012*M* $HClO_4$/satd. $NaClO_4$). Sol. H_2O.

Bis(dithionate): [15038-32-1].
Synth. from *cis*-$[Cr(H_2O)(OH)(en)_2][S_2O_6]$ under reflux in Ac_2O. Red cryst. Insol. H_2O.

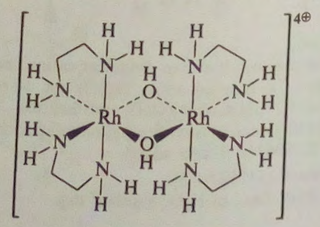
[15135-03-2, 43143-58-4, 51456-44-1, 52542-66-2, 52542-68-4, 57159-02-1, 60363-37-3, 62742-82-9, 64754-05-8, 67392-71-6, 70116-58-4, 70116-59-5, 75598-67-3]

Springborg, J. *et al, Acta Chem. Scand., Ser. A*, 1976, **30**, 171 (*synth, uv, equilibria*)
Cline, S.J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1662 (*cryst struct, magnetism*)
Inorg. Synth., 1978, **18**, 75 (*synth, uv*)
Kaas, K., *Acta Crystallogr., Sect. B*, 1979, **32**, 2021 (*cryst struct*)
Beutler, A. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 983 (*cryst struct, magnetism, uv*)
Christensson, F. *et al, Acta Chem. Scand., Ser. A*, 1980, **34**, 317.
Decurtins, S. *et al, Inorg. Chem.*, 1982, **21**, 1101, 3598 (*uv, magnetism*)

$C_8H_{34}N_8O_2Rh_2^{4\oplus}$ IC-006365

Tetrakis(ethylenediamine)di-μ-hydroxydirhodium(*III*)(4+)

Di-μ-hydroxobis[bis(ethylenediamine)rhodium(III)]



M 480.2 (ion)
Probably bioctahedral as shown with *meso* (ΛΔ) config.

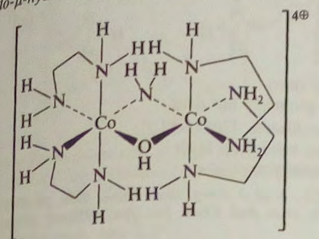
Tetrabromide: Pale yellow solid + $2H_2O$ (H_2O).

Hancock, M. *et al, Acta Chem. Scand., Ser. A*, 1979, **33**, 499; 1982, **36**, 313 (*synth, uv, kinetics*)

$C_8H_{35}Co_2N_9O^{4\oplus}$ IC-006366

μ-Amidotetrakis(ethylenediamine)-μ-hydroxydicobalt(*III*)(4+)

μ-Amido-μ-hydroxobis[bis(ethylenediamine)cobalt(III)](4+)



M 391.2 (ion)
Can be resolved. Formed in redn. of $[en_2Co(NH_2)(O)Coen_2]^{3\oplus}$ by $I^\ominus$. OH bridge can be broken with e.g. H_2O, liq. NH_3.

Tetranitrate: Orange-red cryst. (H_2O).

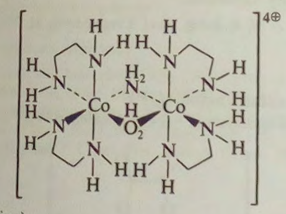
Werner, A., *Ber.*, 1914, **47**, 1961 (*synth, resoln*)
Garbett, K. *et al, J. Chem. Soc., Chem. Commun.*, 1966, 99 (*reactions*)
Davies, R. *et al, J. Chem. Soc. A*, 1968, 2237, 2840 (*synth, reactions*)
Sasaki, Y. *et al, Bull. Chem. Soc. Jpn.*, 1969, **42**, 146 (*synth, cd, uv-vis*)

$C_8H_{35}Co_2N_9O_2^{4\oplus}$ IC-006367

μ-Amidotetrakis(ethylenediamine)-μ-(hydroperoxy)dicobalt(4+), 8CI

μ-Amido(hydroperoxo)bis[bis(ethylenediamine)cobalt(III)]

[23314-47-8]



M 407.2 (ion)
Mode of bridging of $HO_2^\ominus$ not certain.

Tetrabromide: [16871-14-0].
Red solid. Sol. H_2O.

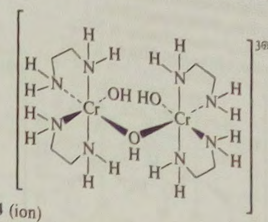
Masayasu, M. *et al, J. Am. Chem. Soc.*, 1967, **89**, 3732 (*synth, uv, kinetics*)

$C_8H_{35}Cr_2N_8O_3^{3\oplus}$ IC-006368

Tetrakis(ethylenediamine)dihydroxy-μ-hydroxydichromium(*III*)(3+)

Tetrakis(1,2-ethanediamine-N,N′)-μ-hydroxydihydroxydichromium(3+), *10CI, 9CI. Hydroxobis[bis(ethylenediamine)hydroxochromium*(III)]

[67392-73-8]



M 395.4 (ion)
Monohydroxy-bridged product formed in reversible ring opening of Tetrakis(ethylenediamine)di-μ-hydroxydichromium(*III*)(4+), IC-006364.

Triperchlorate: [71154-81-9].
Stable red cryst. + $2H_2O$ (0.01*M* NaOH/satd. $NaClO_4$). Reverts to Tetrakis(ethylenediamine)di-μ-hydroxydichromium(*III*)(4+), IC-006364 in 0.12*M* $HClO_4$.

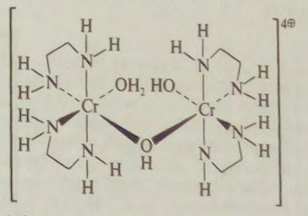
[57159-06-5]

Springborg, J. *et al, Acta Chem. Scand., Ser. A*, 1976, **30**, 171 (*synth, vis, equilibria*)
Kaas, K., *Acta Crystallogr., Sect. B*, 1979, **35**, 1603 (*cryst struct*)
Christensson, F. *et al, Acta Chem. Scand., Ser. A*, 1980, **34**, 317.

$C_8H_{36}Cr_2N_8O_3^{4\oplus}$ IC-006369

Aquatetrakis(ethylenediamine)hydroxy-μ-hydroxydichromium(*III*)(4+)

Aquatetrakis(1,2-ethanediamine-N,N′)-μ-hydroxyhydroxydichromium(III)(4+), *10CI, 9CI*



M 396.4 (ion)
Mono-hydroxy-bridged dinuclear cation with distorted octahedral Cr. In equilibrium with Tetrakis(ethylenediamine)dihydroxy-μ-hydroxydichromium(*III*)(3+), IC-006368, and Tetrakis(ethylenediamine)di-μ-hydroxydichromium(*III*)(4+), IC-006364 in H_2O.

Tetrabromide: [62661-32-9].
Red solid. Meso and racemic-forms identified by ir and cryst struct.

Tetraperchlorate: [57159-08-7].
From Tetrakis(ethylenediamine)dihydroxy-μ-hydroxydichromium(*III*)(3+), IC-006368 in ice-cold 0.6*M* $HClO_4$/satd. $NaClO_4$. Sol. H_2O. Solid gives Tetrakis(ethylenediamine)di-μ-hydroxydichromium(*III*)(4+), IC-006364 (meso-form) slowly at r.t., rapidly at 60°; also on dissolution in H_2O.

▷ Potentially explosive.

[62840-29-3, 75598-68-4]

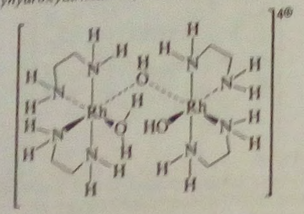
Springborg, J. *et al, Acta Chem. Scand., Ser. A*, 1976, **30**, 171 (*synth, uv, props*)
Christensson, F. *et al, Acta Chem. Scand., Ser. A*, 1980, **34**, 317 (*synth, props, uv*)

IC-006370

$C_6H_{36}N_8O_3Rh_2^{4\oplus}$

Aquatetrakis(ethylenediamine)-μ-hydroxyhydroxydirhodium(*III*)(4+)

Aquatetrakis(1,2-ethanediamine-N,N′)-μ-hydroxyhydroxydirhodium(III)(4+), 11Cl



M 498.2 (ion)
Prob. octahedral struct. shown.
Tetraperchlorate: [83082-99-9].
Sol. H_2O.
Dinitrite, diperchlorate: Red cryst.
Dinitrite, dilodide: [69102-49-4].
Yellow solid.

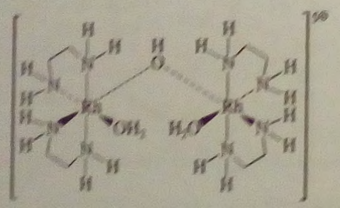
Grenthe, I. *et al, Inorg. Chem.*, 1979, **18**, 1109 (*cryst struct*)
Hancock, M. *et al, Acta Chem. Scand., Ser. A*, 1982, **36**, 313 (*synth, uv, kinetics*)

IC-006371

$C_6H_{37}N_8O_5Rh_2^{5\oplus}$

Diaquatetrakis(ethylenediamine)-μ-hydroxydirhodium(*III*)(5+)

Diaquatetrakis(1,2-ethanediamine-N,N′)-μ-hydroxydirhodium(III)(5+), 11Cl. μ-Hydroxybis[aquabis(ethylenediamine)rhodium(III)]
[83082-97-7]



M 499.2 (ion)
Synth. from $[(en)_2Rh(OH)_2Rh(en)_2]^{4\oplus}$ in acid soln. Not isol.

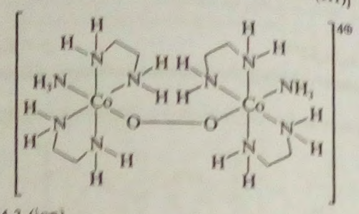
Hancock, M. *et al, Acta Chem. Scand., Ser. A*, 1982, **36**, 313 (*synth, kinetics*)

IC-006372

$C_6H_{38}Co_2N_{10}O_2^{4\oplus}$

Diamminetetrakis(ethylenediamine)-μ-peroxydicobalt(4+)

μ-Peroxobis[amminebis(ethylenediamine)cobalt(III)]



M 424.3 (ion)
Precise geometry not detd.
Tetraperchlorate: [36573-37-2].
Brown solid. Sol. H_2O.
▷ Potentially explosive.

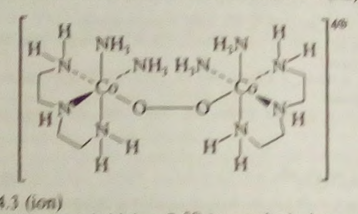
Duffy, D.L. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 2053 (*synth, uv*)
Sasaki, Y. *et al, Bull. Chem. Soc. Jpn.*, 1971, **44**, 3373 (*synth, uv*)

IC-006373

$C_6H_{38}Co_2N_{10}O_2^{4\oplus}$

Tetraamminebis(diethylenetriamine)-μ-peroxydicobalt(*III*)(4+)

μ-Peroxobis[diammine(diethylenetriamine)cobalt(III)](4+)



M 424.3 (ion)
Believed to have bridging $O_2^{2\ominus}$ in octahedral struct, precise geometry not ascertained.
Tetraperchlorate: Brown solid. Sol. H_2O.
▷ Potentially explosive.

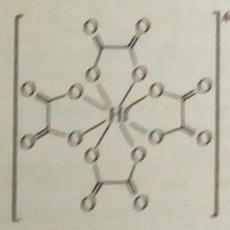
Duffy, D.L. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 2053 (*synth, uv*)

IC-006374

$C_9HfO_{16}^{4\ominus}$

Tetrakis(oxalato)hafnate(*IV*)

Tetrakis(ethanedioato(2−)-O,O′)hafnate(IV)(4−), 11Cl



M 530.5 (ion)
Distorted dodecahedron.
Tetra-Na salt, trihydrate: [60896-78-8].
White solid (H_2O).
Tetra-K salt, pentahydrate: [51716-88-2].
Synth. by reaction between $HfOCl_2.8H_2O$, $K_2C_2O_4$ and $H_2C_2O_4$ in aq. soln. White solid (H_2O).

Inorg. Synth., 1966, **8**, 42 (*synth*)

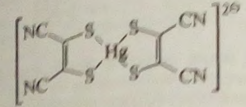
Tranqui, D. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 3126 (*cryst struct, $K_2.5H_2O$ salt*)
Vuillet, P. *et al, Chem. Phys. Lett.*, 1978, **55**, 297 (*quadrupole interaction*)

IC-006375

$C_8HgN_4S_4^{2\ominus}$

Bis(maleonitriledithiolato)mercurate(2−)

Bis(1,2-dicyanoethene-1,2-dithiolato-S,S′)mercurate(2−). Bis(2,3-dimercapto-2-butenedinitrilato(2−)-S,S′) mercurate(2−), 10Cl
[64608-29-3]



M 480.9 (ion)
Bis-tetrabutylammonium salt: [93365-76-5].
1,1′-Dimethyl-4,4′-bipyridinium(2+) salt: [107798-06-1].
Violet needles. Mp 220°.
Bis-Ph_4As salts: [64608-30-6].
Yellow green cryst. Mp 213°.

Stocco, G.C., *Inorg. Chim. Acta*, 1977, **24**, L65 (*synth, ir, Ph_4As salt*)
Inoue, S. *et al, Nippon Kagaku Kaishi (J. Chem. Soc. Jpn.)*, 1981, 1867 (*stability const, anion*)
Fernandez, A. *et al, Chem. Ber.*, 1984, **117**, 3102; 1985, **118**, 1936 (*uv, photochem, Bu_4N salt*)
Leitner, S. *et al, Chem. Ber.*, 1987, **120**, 1011 (*synth, uv, dimethylbipyridinium salt*)

IC-006376

$C_2I_2Mn_2O_8$

Octacarbonyldi-μ-iododimanganese, 9Cl, 8Cl

Di-μ-iodooctacarbonyldimanganese
As Di-μ-bromooctacarbonyldimanganese, IC-005854 with

X = I

M 587.7
Synth. by heating $MnI(CO)_5$ in pet. ether at 100-120°.
Monomer: Tetracarbonyliodomanganese. Iodotetracarbonylmanganese
C_4IMnO_4 M 293.8
Has no separate existence.

Abel, E.W. *et al, J. Chem. Soc.*, 1959, 1501 (*synth, props*)
El-Sayed, M.A. *et al, Inorg. Chem.*, 1963, **2**, 158 (*ir*)
Zingales, F. *et al, Inorg. Chem.*, 1967, **6**, 1243 (*props*)
Fiorani, M.P. *et al, J. Inorg. Nucl. Chem.*, 1967, **29**, 1814 (*synth*)
Bamford, C.H. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1846 (*synth*)

IC-006377

$C_{12}I_2O_{24}Os_4$

Octacarbonyldi-μ-iodotriosmium

[52587-71-9]

$IOs(CO)_4$—$Os(CO)_4I$

M 858.2
Diastl. Synth. from $Os_3(CO)_{12}H_2$ with I_2 in hexane. Precursor of $Os_3(CO)_8I_2$. Air-stable yellow cryst. Sol. polar solvs; spar. sol. non polar solvs. Mp 133-136°. Characterised spectroscopically.

Bruce, M.I. *et al, J. Chem. Soc. A*, 1969, 987 (*synth, ir*)
Johns, E.E. *et al, Inorg. Chim. Acta*, 1983, **70**, 207 (*use*)
Geoffroy, G.L. *et al, Inorg. Chem.*, 1986, **25**, 2916 (*synth*)
Rosa, J.R. *et al, Inorg. Chim. Acta*, 1988, **147**, 251 (*cryst struct*)
Inorg. Synth., 1989, **25**, 187 (*synth*)

IC-006378

$C_8I_2O_8Tc_2$

Octacarbonyldi-μ-iododitechnetium

Diiodooctacarbonylditechnetium. Iodotetracarbonyltechnetium dimer
[19583-91-6]

As Di-μ-bromooctacarbonylditechnetium, IC-005856 with

X = I

M 675.7
Synth. from $Tc_2(CO)_{10}$ and I_2 in a sealed ampoule. $Te(CO)_5I$ precursor. Diamagnetic solid.

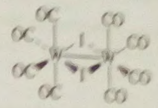
Hileman, J.C. *et al, J. Am. Chem. Soc.*, 1961, **83**, 2953 (*synth, ir*)
Hileman, J.C. *et al, Inorg. Chem.*, 1962, **1**, 933 (*synth, ir*)
El-Sayed, M.A. *et al, Inorg. Chem.*, 1963, **2**, 158 (*ir*)
Orgel, L.E., *Inorg. Chem.*, 1964, **3**, 303 (*ir*)

IC-006379

$C_8I_2O_8W_2$

Octacarbonyldi-μ-iododitungsten, 9Cl

[55405-97-5]



M 845.5
W—W bond length 315.5 pm.

Schmid, G. *et al, Chem. Ber.*, 1975, **108**, 260; 1976, **109**, 2148 (*synth, props, cryst struct*)

IC-006380

C_8K

Potassium graphite (KC_8), 9Cl

Potassium compd. with graphite (1:8), 11Cl, 10Cl. Potassium-graphite intercalate. Potassium-graphite lamellar compound
[12081-88-8]

C_8K

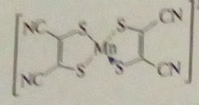
M 135.1
Member of a series of compds ($C_{24}K$, $C_{36}K$, $C_{48}K$, $C_{60}K$, $C_{72}K$) formed by intercalation of potassium into the graphite layer lattice struct. Synth. either by reaction of K vapour with graphite at 300°, by electrolysis of fused K salts with graphite electrodes or by reaction of graphite with solns. of K in liq. NH_3. Becomes superconducting at 0.14K, forms intercalation compds. with H_2 (C_8KH_2) or C_8KD_2). Powerful reducing agent. Bronze powder with metallic appearance. Moisture-sensitive. Reacts with H_2O_2, leaching out potassium as KOH.

Billaud, D. *et al, Carbon '76 Int. Carbon Conf., Preprr. Ind.*, 1976, 135; *C.A.*, 1977, **86**, 182222 (*synth*)
Lagrange, P. *et al, Proc. London Int. Carbon, Graphite Conf., 5th*, 1978, **2**, 660; *C.A.*, 1980, **93**, 224646 (*struct*)
Howarth, D.T. *et al, J. Solid State Chem.*, 1980, **31**, 345 (*use*)
Tamura, T. *et al, J. Chem. Soc., Faraday Trans. 1*, 1982, **78**, 2369 (*struct, hydrogen intercalation*)
Takada, Y., *J. Phys. Soc. Jpn.*, 1982, **51**, 63 (*superconductivity*)
Selivanov, S.I. *et al, Dop. Khim.*, 1986, **95**, 340 (*use*)

$C_8MnN_2S_4^{2\ominus}$ IC-006381

Bis(maleonitriledithiolato)manganate(*II*)(2−)

Bis(dimercaptomaleonitrilato(2−))manganate(2−), 8Cl. Bis(dimercaptomaleonitrilato)manganate(2−) Bis(cis-1,2-dicyano-1,2-ethenedithiolato)manganate(2−)



M 335.3 (ion)

May have tetrahedral geometry as suggested for similar dithiooxalate complexes and found for a 1,2-*p*-toluenedithiolate complex.

Bis-Et_4N salt: [20584-89-8].

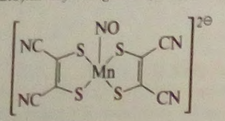
Synth. by addition of aq. $MnCl_2{\cdot}4H_2O$ to a soln. of $[Et_4N]Cl$ and $Na_2S_2C_2(CN)_2$ under N_2. Air-sensitive light brown cryst. Sl. sol. Me_2CO.

McCleverty, J.A. *et al, J. Chem. Soc. A*, 1968, 816 (*synth*)
Coucouvanis, D. *et al, Inorg. Chem.*, 1975, **14**, 2657, 6917 (*struct*)
Henkel, G. *et al, Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 117 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 39 (*rev, bibl*)

$C_8MnN_2OS_4^{2\ominus}$ IC-006382

Bis(maleonitriledithiolato)(nitrosyl)manganate(2−)

*Bis[2,3-dimercapto-2,3-butenedinitrilato(2−)-S,S′] nitrosylmanganate(2−). Bis(*cis*-1,2-dicyano-1,2-ethenedithiolato)nitrosylmanganate(2−)*



M 365.3 (ion)

Geometry not known.

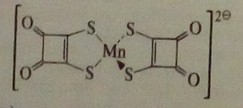
Bis-Et_4N salt: Synth. by bubbling NO through degassed aq. EtOH soln. of hydrated $MnCl_2$, addition of $Na_2S_2C_2N_2$, and treatment with $[Et_4N]Br$. Green-black cryst., unstable in air. Sol. polar org. solvs., CH_2Cl_2; insol. 2-propanol, pentane. Mp 218-220°.

James, T.A. *et al, J. Chem. Soc. A*, 1970, 3318 (*synth, ir, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 44 (*rev, bibl*)

$C_8MnO_4S_4^{2\ominus}$ IC-006383

Bis[3,4-dimercapto-3-cyclobutene-1,2-dionato(2−)-*S,S′*] manganate(*II*)(2−), 9Cl

Bis(dithiosquarato-S,S′)manganate(II)(2−)



M 343.2 (ion)

Magnetic data suggest tetrahedral MnS_4.

Di-K salt: [56488-47-2].

Synth. from stoichiometric quantities of $MnCl_2$ and $K_2[C_4O_2S_2]$ in H_2O under N_2. Air-sensitive yellow cryst. + $4H_2O$ (H_2O). $\mu_{eff} = 6.13\mu_B$.

Bis-Ph_4P salt: [56488-41-6].

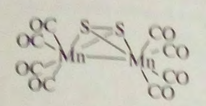
Synth. from stoichiometric amounts of $MnCl_2$, $K_2[C_4O_2S_2]$ and $[Ph_4P]Cl$ in H_2O under N_2. Yellow cryst. (MeCN or CH_2Cl_2 after vacuum drying of dihydrate). Insol. H_2O. Mp 232° dec. $\mu_{eff} = 5.87\mu_B$.

Coucouvanis, D. *et al, Inorg. Chem.*, 1975, **14**, 2657 (*synth, cryst struct, ir, uv, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 40 (*rev, bibl*)

$C_8Mn_2O_8S_2$ IC-006384

Octacarbonyldi-μ-thioxodimanganese, 9Cl

[54936-08-2]



M 398.0

Diamagnetic; struct. uncertain. Synth. from $Mn_2(CO)_{10}$ and bis(fluorocarbonyl)disulfane in C_6H_6. Air-sensitive golden-yellow cryst. (C_6H_6). Mp 128°. Ir ν_{CO} 2098w, 2068vs, 2015s, 1991m cm^{-1} (cyclohexane).

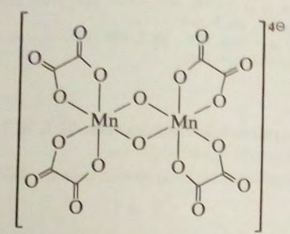
Chaudhuri, M.K. *et al, J. Organomet. Chem.*, 1975, **85**, 85 (*synth, ir*)

$C_8Mn_2O_{18}^{4\ominus}$ IC-006385

Tetrakis(oxalato)di-μ-oxodimanganate(*IV*)(4−)

Tetrakis[ethanedioato(2−)-O,O′]di-μ-oxodimanganate(4−), 9Cl

[57628-77-0]



M 493.9 (ion)

Synth. from oxalic acid and $KMnO_4$ at 0°.

Tetra-K salt: [55188-89-1].

Green cryst. + $4H_2O$ (0.1*M* oxalic acid/EtOH); stable for *ca.* one week in the dark at −6°. Barium and $[CoCl(NH_3)_5]^{2\oplus}$ salts are also known.

Cartledge, W.P. *et al, J. Am. Chem. Soc.*, 1936, **58**, 2069 (*synth, uv*)
Grey, J.T., *J. Am. Chem. Soc.*, 1946, **68**, 605 (*magnetism*)
Yoshino, Y. *et al, Bull. Chem. Soc. Jpn.*, 1974, **47**, 2787 (*synth, uv, ir, magnetism, struct*)
Uehiro, T. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 2809 (*dec*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 122 (*rev, bibl*)

$C_8MoN_8^{4\ominus}$ IC-006386

Octakis(cyano-*C*)molybdate(*IV*)(4−), 11Cl, 10Cl, 9Cl

Octacyanomolybdate(IV)(4−)

[17923-49-8]

$[Mo(CN)_8]^{4\ominus}$

M 304.0 (ion)

Depending on counter cation, anion is dodecahedral or approaches 4,4-bicapped trigonal prism or square antiprism. Mo—C_{av} 215.9, C—N_{av} 115.0 pm. Diamagnetic. Many salts.

Tetra-Li salt: [39708-88-8].

Tetra-K salt: [17457-89-5].

Orange cryst. + $2H_2O$.

Di-cyanium, bis-Et_3NH salt: [73307-58-1].

Yellow cryst.

Tetrakis(2-carboxypyridinium) salt: [75261-69-7].

Orange cryst.

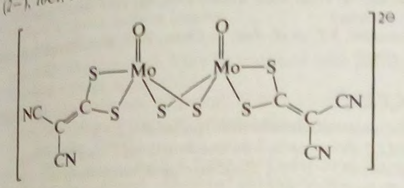
[17450-18-7, 17594-64-8]

Mastterties, E.L., *Inorg. Chem.*, 1973, **9**, 1963 (*cmr*)
Zubritskaya, D.I. *et al, Koord. Khim.*, 1977, **3**, 866; *C.A.* **87**, 61897 (*synth*)
Basson, S.S. *et al, Acta Crystallogr., Sect. B*, 1980, **36**, 2025 (*cryst struct, synth*)
Leipoldt, J.G. *et al, Inorg. Chim. Acta*, 1980, **44**, L99 (*cryst struct, cyanium salt*)
Hahn, E. *et al, J. Mol. Struct.*, 1981, **77**, 165 (*ir, raman*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 1345 (*rev*)

$C_8Mo_2N_4O_2S_6^{2\ominus}$ IC-006387

Bis(1,1-dicyano-2,2-ethylenedithiolato)dioxodi-μ-sulfidodimolybdate(*V*)(2−)

Di-μ-sulfidobis[oxo-1,1-dicyano-2,2-ethylenedithiolatomolybdate(V)]. *Bis[(dimercaptomethylene) propanedinitrilato(2−)-S,S′]dioxodi-μ-thioxodimolybdate*(V)(2−), *10Cl, 9Cl*



M 568.3 (ion)

Distorted square pyramids with O atom in axial position and *cis*-bent $Mo_2O_2S_2^{2\oplus}$ core. Ir $\nu_{Mo-O,S}$ 970s, 955m; ν_{MoSMo} 485m, 345m cm^{-1}.

Di-K salt: [66322-51-8].

Yellow cryst.

Bis-tetrabutylammonium salt: [59389-04-7].

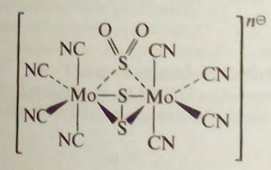
Yellow air-stable cryst. (Me_2CO/EtOH).

Gelder, J.I. *et al, Inorg. Chem.*, 1976, **15**, 1839 (*cryst struct*)
Brant, P. *et al, J. Less-Common Met.*, 1977, **54**, 81 (*pe*)
Schultz, F.A. *et al, Inorg. Chem.*, 1978, **17**, 1758 (*synth, props*)

$C_8Mo_2N_8O_2S_3^{4\ominus}$ IC-006388

Octakis(cyano-*C*)[μ-(disulfur-*S,S′:S,S′*)]-μ-sulfonyldimolybdate(*IV*)(4−), 11Cl, 10Cl

μ-Sulfonyl-μ_4-dithiooctacyanodimolybdate(IV)(4−)



$n = 4$

M 528.2 (ion)

Approx. pentagonal bipyramidal at Mo. First complex in which SO_2 and $S_2^{2\ominus}$ have a mutually bridging role. Diamagnetic.

Tetra-K salt: [89975-10-0].

Black-violet cryst. Mo—Mo distance 268.4 pm. Forms mixed cryst. with paramagnetic $5^{\ominus}$ ion.

Tetrakis-Ph_4P salt: [75899-74-0].

Purple cryst. + $6H_2O$. Mo—Mo distance 273.0 pm, suggesting possible metal-metal bond.

[92842-13-2]

Potvin, C. *et al, J. Chem. Soc., Chem. Commun.*, 1980, 664 (*synth, ir, cryst struct*)
Müller, A. *et al, Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 389 (*synth, cryst struct*)
Manoli, J.M. *et al, Inorg. Chim. Acta*, 1984, **88**, 75 (*ir, synth, cryst struct*)

$C_8Mo_2N_8O_2S_3^{5\ominus}$ IC-006389

Octakis(cyano-*C*)[μ-(disulfur-*S,S′:S,S′*)]-μ-sulfonyldimolybdate(*III, IV*)(5−), 11Cl

As Octakis(cyano-*C*)[μ-(disulfur-*S,S′:S,S′*)]-μ-sulfonyldimolybdate(*IV*)(4−), IC-006388 with

$n = 5$

M 528.2 (ion)

Approx. pentagonal bipyramidal struct. Formed as mixed cryst. with Octakis(cyano-*C*)[μ-(disulfur-*S,S′:S,S′*)]-μ-sulfonyldimolybdate(*IV*)(4−), IC-006388. Mo—Mo 279 pm.

Penta-K salt: [89975-11-1].

Black-violet cryst. Paramagnetic.

Müller, A. *et al, Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 389 (*synth, cryst struct, pe, esr, uv, ir*)

$C_8Mo_2N_8S_2^{4\ominus}$ IC-006390

Octakis(cyano-*C*)di-μ-thioxodimolybdate(*IV*)(4−), 11Cl

Bis[μ_2-sulfido]octacyanodimolybdate(IV)

M 464.1 (ion)

Pseudo-octahedral coordination of Mo atoms. MoS_2Mo unit is planar. Interatomic distances: Mo—Mo 275.8, Mo—S_{ax} 229.6, Mo—C_{ax} 212 pm.

Tetrakis-Ph_4P salt: [97278-56-3].

Green solid or bluish green cryst. + $2H_2O$.

[97278-61-0]

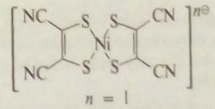
Muller, A. *et al, Inorg. Chem.*, 1985, **24**, 2872 (*cryst struct, synth, uv-vis, raman, ir, pe*)

$C_8N_4NiS_4^{\ominus}$ IC-006391

Bis(maleonitriledithiolato)nickelate(1−)

Bis(dimercaptomaleonitrilato)nickelate(1−), 8Cl. Bis(2,3-dimercapto-2-butenedinitrilato)nickelate(1−)

[13964-77-7]



$n = 1$

M 339.0 (ion)

Forms many salts, most having structs. with stacks of anions. Salts with planar cations exhibit important electrical conductance caused by stacks of alternating cations and anions.

Et_4N salt: Black needles. Sol. polar org. solvs.

Tetrathiafulvalenenickel salt: [52700-52-4].

$C_{14}H_4N_4NiS_8$ M 543.4

Electrical conducivity 10^5 times higher than $Na[Ni[S_2C_2(CN)_2]_2]$. Black cryst. (Me_2CO). Believed to be ionic.

[46761-25-5]
Wudl, F. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 923 (*synth, esr, conductivity deriv*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 177; **6**, 147.

$C_8N_4NiS_4^{2\ominus}$ IC-006392

Bis(maleonitriledithiolato)nickelate(2−)
Bis(dimercaptomaleonitrilate)nickelate(2−), 8CI. Bis(2,3-dimercapto-2-butenedinitrilato)nickelate(2−), 9CI
[14876-79-0]
As Bis(maleonitriledithiolato)nickelate(1−), IC-006391 with

n = 2

M 339.0 (ion)
Forms many salts, most having structs. with stacks of anions, or stacks of alternating cations and anions.
Bis-Et_4N salt: [15665-90-4].
Orange-red cryst. Sol. $MeNO_2$. Mp 143-145°.
Bis-tetrabutylammonium salt: [18958-57-1].
$C_{40}H_{72}N_6NiS_4$ M 824.0
Green-gold solid. Sol. DMF, MeCN. Mp 191-192°.
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 177; **6**, 147.

$C_8N_4NiS_4^{3\ominus}$ IC-006393

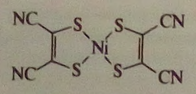
Bis(maleonitriledithiolato)nickelate(3−)
Bis(dimercaptomaleonitrilato)nickelate(3−), 8CI. Bis(2,3-dimercapto-2-butenedinitrilato)nickelate(3−), 9CI
[38117-63-4]
As Bis(maleonitriledithiolato)nickelate(1−), IC-006391 with

n = 3

M 339.0 (ion)
Formed in soln. by reduction of Bis(maleonitriledithiolato) nickelate(2−), IC-006392 but no solids isol. Green soln. Sol. MeCN.
Geiger, W.E. *et al, Inorg. Chem.*, 1977, **16**, 2003.

$C_8N_4NiS_4$ IC-006394

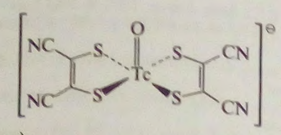
Bis(maleonitriledithiolato)nickel
Bis(dimercaptomaleonitrilato)nickel, 8CI. Bis(2,3-dimercapto-2-butene dinitrilato-S,S) nickel, 9CI
[19280-13-8]



M 339.0
Struct. not determined. Obt. by electrochem. oxidn. of monoanion Bis(maleonitriledithiolato)nickelate(1−), IC-006391, but this may really be ligand oxidation rather than Ni.
Fanghaenel, E. *et al, Z. Chem.*, 1979, **19**, 192 (*synth*)
Persaud, L. *et al, Inorg. Chem.*, 1985, **24**, 3562 (*electrochem*)

$C_8N_4OS_4Tc^{\ominus}$ IC-006395

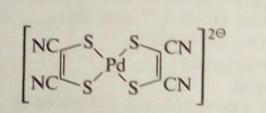
Bis(maleonitriledithiolato)oxotechnetate(V)(1−)
Bis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S']oxotechnetate(1−), 11CI. Bis(1,2-dicyanoethenedithiolato)oxotechnetate(V)(1−)



M 395.2 (ion)
Square pyramidal anion. Prep. from $[TcOCl_4]^{\ominus}$ or from Tc^{V}-gluconate + ligand.
Et_4N salt: [70317-72-5].
Red solid (aq. EtOH). Mp 180-182°.
Ph_4As salt: Red-brown cryst. Mp 156-159°.
Spies, H. *et al, Inorg. Chim. Acta*, 1979, **33**, L113; 1981, **48**, 255 (*synth, ir, uv, ms, pmr*)
Davison, A. *et al, Inorg. Chem.*, 1980, **19**, 1988 (*ir, uv, electrochem*)
Abram, U. *et al, Z. Chem.*, 1984, **24**, 74 (*synth, ir, uv*)
Görner, W. *et al, Anal. Chem.*, 1986, **58**, 1261 (*anal, γ-ray spectrosc*)
Colmanet, S.F. *et al, Aust. J. Chem.*, 1988, **41**, 151 (*synth, ir, cryst struct*)

$C_8N_4PdS_4^{2\ominus}$ IC-006396

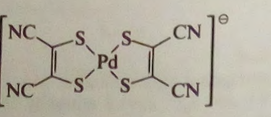
Bis(maleonitriledithiolato)palladate(2−)
Bis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S'] palladate(2−), 9CI. Bis[dimercaptomaleonitrilato(2−)] palladate(2−), 8CI
[19555-33-0]



M 386.7 (ion)
Synth. from $PdCl_2$ + the di-Na salt of the ligand.
Bis-Et_4N salt: [15665-98-2].
Green platelets. Mp ~240° dec.
Bis-tetrabutylammonium salt: [18958-59-3].
Green platelets. Mp 157-158°.
Billig, E. *et al, Inorg. Chem.*, 1964, **3**, 663 (*synth, ir*)
Weiher, J.F. *et al, J. Am. Chem. Soc.*, 1964, **86**, 4329 (*synth*)
Inorg. Synth., 1967, **10**, 8 (*synth*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1968, 1299 (*ir*)

$C_8N_4PdS_4^{\ominus}$ IC-006397

Bis(maleonitriledithiolato)palladate(1−)
Bis[dimercaptomaleonitrilato(2−)]palladate(1−), 8CI. Bis[2,3-dimercapto-2-butenedinitrilato(2−)]palladate(1−), 9CI
[19570-29-7]

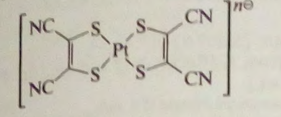


M 386.7 (ion)
Anions can form stacked struct. Not so well studied as Ni, Pt analogues. Synth. from $Na_2(C_4N_2S_2)$ and $Pd(NH_3)_4Cl_2$. Sol. DMF.
Et_4N salt: [21328-88-1].
No phys. props. reported. Diamagnetic.
Tetrabutylammonium salt: [19333-23-4].

Billig, E. *et al, Inorg. Chem.*, 1964, **3**, 663 (*synth, sol struct*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1968, 1299 (*ir*)
Kirmse, R. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 255 (*esr*)
Perez-Albuerne, E.A. *et al, J. Chem. Soc., Chem. Commun.*, 1977, 417 (*electrochem*)
Persaud, L. *et al, Inorg. Chem.*, 1985, **24**, 3562 (*uv, electrochem*)

$C_8N_4PtS_4^{\ominus}$ IC-006398

Bis(maleonitriledithiolato)platinate(1−)
Bis(dimercaptomaleonitrilato)platinate(1−), 8CI. Bis(2,3-dimercapto-2-butenedinitrilato)platinate(1−), 9CI
[14977-45-8]



n = 1

M 475.4 (ion)
Many studies of solid state electric conductance of stacked structures, particularly of partly-oxidised compounds. Salts of organic cations known.
Li salt: [82489-50-7].
Not fully characterised. May be confused with partially oxidised Li salt. Black solid.
Li salt (partly oxidised), dihydrate: [77812-45-4]. *LiPt(mnt)*
Black needles and plates. Formulated as $Li_{0.75}Pt(mnt)_2.2H_2O$.
Rb salt: Black solid. Distinct from partly oxidised Rb salt.
Rb salt (partly oxidised), dihydrate: [93267-33-5].
Black solid. Formulated as $Rb_{0.8}Pt(mnt)_2.2H_2O$.
Et_4N salt: [15711-74-7].
Black solid. Mp 288° dec.
Tetrabutylammonium salt: [55529-88-9].
Black solid.
[83854-40-4]
Davison, A. *et al, Inorg. Chem.*, 1963, **2**, 1227 (*synth, uv, esr*)
Inorg. Synth., 1967, **10**, 19 (*synth*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1968, 1299 (*ir*)
Grim, S.O. *et al, Inorg. Chem.*, 1974, **13**, 447 (*pe*)
Ahmad, M.M. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1759 (*struct, elec cond*)
Underhill, A.E., *Compr. Coord. Chem.*, Pergamon, Oxford, 1987, **6**, 148.

$C_8N_4PtS_4^{2\ominus}$ IC-006399

Bis(maleonitriledithiolato)platinate(2−)
Bis(dimercaptomaleonitrilato)platinate(2−), 8CI. Bis(2,3-dimercapto-2-butenedinitrilato)platinate(2−), 9CI
[15152-99-5]
As Bis(maleonitriledithiolato)platinate(1−), IC-006398 with

n = 2

M 475.4 (ion)
Many studies of charge delocalisation and electric conductance in solid. Salts of organic cations known.
Bis-Et_4N salt: [15711-73-6].
Dark red cryst. Mp 242-245° dec.
Inorg. Synth., 1967, **10**, 19 (*synth*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1968, 1299 (*ir*)
Grim, S.O. *et al, Inorg. Chem.*, 1974, **13**, 447 (*pe*)
Clark, R.J.H. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 2142 (*uv, raman*)
Ahmad, M.M. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 165 (*uv, elec cond*)

$C_8N_4PtS_4^{4\ominus}$ IC-006400

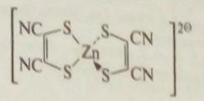
Bis(maleonitriledithiolato)platinate(4−)
Bis(2,3-dimercapto-2-butenedinitrilato)platinate(4−), 9CI
[62906-12-1]
As Bis(maleonitriledithiolato)platinate(1−), IC-006398 with

n = 4

M 475.4 (ion)
Formed by reduction of analogous (2−) anion, Bis(maleonitriledithiolato)platinate(2−), IC-006399, but not isol.
Geiger, W.E. *et al, Inorg. Chem.*, 1977, **16**, 2003.

$C_8N_4S_4Zn^{2\ominus}$ IC-006401

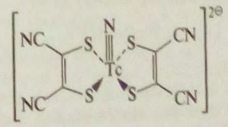
Bis(maleonitriledithiolato)zincate(2−)
(cis-1,2-Dicyano-1,2-ethylenedithiolato)zincate(2−). Bis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S']zincate(2−), 9CI
[41139-14-4]



M 345.7 (ion)
Bis-Et_4N salt: [21312-70-9].
Cryst.
Bis-tetrabutylammonium salt: [18958-61-7].
Catalyses photo-production of H_2 from H_2O. Pale yellow needles (aq. EtOH). Mp 156-158°.
1,1'-Dimethyl-4,4'-bipyridinium(2+) salt: [97251-94-0].
Red cryst. Mp 270° dec.
Bis-Ph_4As salt: [101078-22-2].
Yellow cryst.
Billig, E. *et al, Inorg. Chem.*, 1964, **3**, 663 (*synth, powder struct*)
Inorg. Synth., 1967, **10**, 8 (*synth, Bu_4N salt*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1968, 1299 (*ir*)
Dance, I.G. *et al, J. Am. Chem. Soc.*, 1973, **95**, 7256 (*synth, uv, pyridinium salts*)
Fernandez, A. *et al, Chem. Ber.*, 1984, **117**, 3102 (*photophys, photochem, Bu_4N salt*)
Fernandez, A. *et al, Chem. Ber.*, 1985, **118**, 1936 (*synth, dimethylbipyridinium salt*)
Stach, J. *et al, Inorg. Chem.*, 1986, **25**, 1369 (*synth, cryst struct, Ph_4As salt*)
Lahner, S. *et al, Chem. Ber.*, 1987, **120**, 1011 (*cryst struct, ir, uv-vis*)

$C_8N_5S_4Tc^{2\ominus}$ IC-006402

Bis(maleonitriledithiolato)nitridotechnetate(V)(2−)
Bis(1,2-dicyanoethenedithiolato)nitridotechnetate(V). Bis[2,3-dimercapto-2-butenedinitrilato(2−)-S,S'] nitridotechnetate(2−), 11CI
[96241-89-3]



M 393.2 (ion)
Square-pyramidal anion. Synth. from $TcNCl_4^{\ominus}$ + Na_2L in EtOH.
Bis-Et_4N salt: [99449-61-3].
Yellow cryst. (Me_2CO/2-propanol). Mp 167-168°.
Bis-Ph_4As salt: [123050-02-2].
Bright yellow cryst. (MeCN). Mp 267-268°.

Abram, U. *et al, Inorg. Chim. Acta*, 1985, **109**, L9 (*synth, ir, nmr, esr*)
Abram, U. *et al, Z. Anorg. Allg. Chem.*, 1987, **544**, 167 (*synth, ir, nmr*)
Williams, G.A. *et al, Aust. J. Chem.*, 1989, **42**, 875 (*synth, ir, cryst struct*)
Baldas, J. *et al, J. Nucl. Med.*, 1989, **30**, 1240 (*hplc, biodistribn*)

IC-006403

$C_8N_8Nb^{5\ominus}$
Octakis(cyano-*C*)niobate(*III*)(5−), 10CI
Octacyanoniobate(III)(*5*−)

$[Nb(CN)_8]^{5\ominus}$

M 301.0 (ion)
Dodecahedral with Nb—C 228.2 (×4), 224.2 (×4) pm. Cmr, ir and Raman spectra suggest a different struct. in soln. probably with D_{4d} symmetry (square antiprism).
Penta-K salt: [59052-55-0].
Synth. by photolysis of $K_4Nb(CN)_8$ in KOH at 647 nm or by reducing $K_4Nb(CN)_8$ with K/Hg in H_2O. Deep red solid (H_2O).
Kiernan, P.M. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 2489 (*synth, ir, raman, esr*)
Hursthouse, M.B. *et al, J. Chem. Soc., Chem. Commun.*, 1980, 1167 (*synth, cryst struct, ir, raman, cmr*)

IC-006404

$C_8N_8Nb^{4\ominus}$
Octakis(cyano-*C*)niobate(*IV*)(4−), 10CI
Octacyanoniobate(IV)(*4*−)
[61055-93-4]

$[Nb(CN)_8]^{4\ominus}$

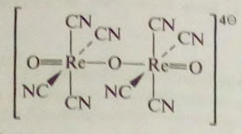
M 301.0 (ion)
Dodecahedral anion in solid state. Esr and ir spectra suggest a square antiprismatic struct. in soln. See also Octakis(cyano-*C*)niobate(*III*)(5−), IC-006403.
Tetra-K salt: [59030-57-8].
Synth. by electrolytic reduction of $NbCl_5$ in MeOH and adding conc. aq. KCN. Orange cryst. + $2H_2O$. Paramagnetic, $\mu_{eff} = 1.69\mu_B$ (290K). Other alkali metal salts also known.
Tetra-Tl(I) salt: [59052-56-1].
$C_8N_8NbTl_4$ M 1118.5
Synth. by adding TlOAc to an aq. soln. of the K-salt. Deep pink solid.
[51341-09-4]
Kiernan, P.M. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 816 (*synth*)
Kiernan, P.M. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 2489.
Griffiths, W.P. *et al, J. Mol. Struct.*, 1978, **46**, 307 (*ir, raman*)
Laing, M. *et al, Inorg. Chim. Acta*, 1979, **33**, L119 (*cryst struct*)

$C_8N_8NpS_8^{4\ominus}$ IC-006405
Octakis(thiocyanato-*N*)neptunate(*IV*)(4−)
Octakis(isothiocyanato)neptunate(IV)(*4*−)

$[Np(NCS)_8]^{4\ominus}$

M 701.7 (ion)
Tetrakis-Et_4N salt: [38356-75-1].
Pale brown cryst. Sol. MeCN, Me_2CO, $MeNO_2$. 8-Coord., cubic, isostructural with U analogue. Ir ν_{C-N} 2045 cm^{-1}.
Al-Kazzaz, Z.M.S. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2273 (*synth, ir*)

$C_8N_8O_3Re_2^{4\ominus}$ IC-006406
Octakis(cyano-*C*)-μ-oxodioxodirhenate(4−)
Octacyano-μ-oxodioxorhenate(*4*−), *8CI*
Octacyanotrioxodirhenate(*4*−)



M 628.5 (ion)
Bi-octahedral with Re═O 169.8, Re—O 191.5, Re—C_{mean} 212 pm.
Tetra-K salt: [26202-03-9].
Synth. from $K_3[ReO_2(CN)_4]$ and HCl aq. Purple needles (EtOH aq.).
Bis[tetraammineplatinum(II)*] salt:*
$C_8H_{24}N_{16}O_3Pt_2Re_2$ M 1154.9
Synth. from K salt and $Pt(NH_3)_4Cl_2$ in H_2O.
Toppen, D.L. *et al, Inorg. Nucl. Chem. Lett.*, 1970, **6**, 139 (*synth, props*)
Shandles, R. *et al, Inorg. Chem.*, 1971, **10**, 2785 (*synth, cryst struct*)

$C_8N_8PaS_8^{4\ominus}$ IC-006407
Octakis(thiocyanato-*N*)protactinate(*IV*)(4−)
Octakis(isothiocyanato)protactinate(IV)(*4*−)

$[Pa(NCS)_8]^{4\ominus}$

M 695.7 (ion)
Tetrakis-Et_4N salt: [38356-73-9].
Solid. Sol. MeCN, $MeNO_2$, Me_2CO. 8-Coord. cubic struct., isostructural with U analogue. Ir ν_{C-N} 2042 cm^{-1}.
Al-Kazzaz, Z.M.S. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2273 (*synth, ir*)

$C_8N_8PrS_8^{5\ominus}$ IC-006408
Octakis(thiocyanato-*N*)praseodymate(*III*)(5−)
Octaisothiocyanatopraseodymate(III)(*5*−)

$[Pr(NCS)_8]^{5\ominus}$

M 605.5 (ion)
Geometry at Pr intermed. between cube and square antiprism.
Pentakis-Me_4N salt: [127778-12-5].
Pale green cryst. + C_6H_6. Sol. MeOH. Similar compds. obt. for La—Dy. Ir ν_{C-N} 2060 cm^{-1}. Stable at 110°.
Matsumura, N. *et al, Bull. Chem. Soc. Jpn.*, 1990, **63**, 620 (*synth, cryst struct, ir, thermal anal*)

$C_8N_8PuS_8^{4\ominus}$ IC-006409
Octakis(thiocyanato-*N*)plutonate(*IV*)(4−)
Octakis(isothiocyanato)plutonate(IV)(*4*−)

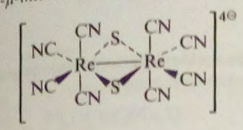
$[Pu(NCS)_8]^{4\ominus}$

M 703.7 (ion)
Tetra-Cs salt: [38832-13-2].
Brown solid. Sol. $MeNO_2$, Me_2CO, H_2O. Believed to be 8-coord., square antiprismatic by analogy with corresp. U compd.
Tetrakis-Et_4N salt: [38832-12-1].

Cryst. Sol. MeCN, $MeNO_2$, Me_2CO. 8-Coord. cubic, isomorphous wih U analogue. Ir ν_{C-N} 2055 cm^{-1}.
Al-Kazzaz, Z.M.S. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2273 (*synth, ir*)
Bombieri, G. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1520 (*cryst struct*)

IC-006410

$C_8N_8Re_2S_4^{4\ominus}$
Octakis(cyano-*C*)di-μ-thioxodirhenate(*IV*)(4−), 10CI
Octacyanodi-μ-thiodirhenate(IV)(*4*−)



M 644.6 (ion)
Tetra-Cs salt: [69290-59-1].
Synth. via treatment of aq. $ReO_4^{\ominus}$ in excess $CN^{\ominus}$ with H_2S followed by precipitation with CsCl. Blue cryst.
Tetrakis-Ph_4P salt: [69290-61-5].
Synth. via treatment of aq. $ReO_4^{\ominus}$ in excess $CN^{\ominus}$ with H_2S followed by precipitation with PPh_4Cl. Deep blue cryst. + $6H_2O$ (MeOH aq. under N_2).
Tetrakis-Ph_4As salt: [69290-62-6].
Synth. via treatment of aq. $ReO_4^{\ominus}$ in excess $CN^{\ominus}$ with H_2S followed by precipitation with Ph_4AsCl. Blue cryst.
Laing, M. *et al, Inorg. Chim. Acta*, 1978, **26**, L27 (*synth, cryst struct*)
Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 1411 (*synth, ir, raman*)

$C_8N_8Re_2S_8^{2\ominus}$ IC-006411
Octakis(thiocyanato-*N*)dirhenate(*III*)(2−), 9CI
Octa(isothiocyanato)dirhenate(III)(*2*−), *8CI*
[48076-42-2]

$[(SCN)_4ReRe(NCS)_4]^{2\ominus}$

M 837.0 (ion)
Assumed to be N-bonded.
Bis-tetrabutylammonium salt: [16591-28-9].
Synth. from $(Bu_4N)_2Re_2Cl_8$ and NaSCN in MeOH/HOAc or in THF. Red cryst. (MeCN). Sol. THF, MeCN, Me_2CO, $MeNO_2$. Sl. sol. EtOH. Insol. H_2O, Et_2O, $CHCl_3$, C_6H_6.
Bis-Ph_3MeAs salt: Dark red cryst.
Bis-Ph_4As salt: [41880-58-4].
Synth. from $(Bu_4N)_2Re_2Cl_8$ and NaSCN in MeOH/HOAc, followed by addn. of Ph_4AsCl. Orange plates. Sol. MeCN, Me_2CO, $MeNO_2$. Sl. sol. THF. Insol. H_2O, EtOH, Et_2O, $CHCl_3$, C_6H_6.
Cotton, F.A. *et al, Inorg. Chem.*, 1967, **6**, 929 (*synth, ir, uv, magnetism*)
Nimry, T. *et al, Inorg. Chem.*, 1977, **16**, 2829 (*synth, ir, uv, struct, props*)

$C_8N_8Re_2Se_8^{2\ominus}$ IC-006412
Octakis(selenocyanato-*N*)dirhenate(*III*)(2−), 9CI
Octa(isoselenocyanato)dirhenate(III)(*2*−), *8CI*

$[(SeCN)_4ReRe(NCSe)_4]^{2\ominus}$

M 1212.2 (ion)
Assumed to be N-bonded.
Bis-tetrabutylammonium salt: [36813-06-6].
Purple cryst.
Cotton, F.A. *et al, Inorg. Chem.*, 1967, **6**, 929 (*synth, props*)
Hendriksma, R.R., *J. Inorg. Nucl. Chem.*, 1972, **34**, 1581 (*synth, ir, props*)

$C_8N_8S_8Th^{4\ominus}$ IC-006413
Octakis(thiocyanato-*N*)thorate(*IV*)(4−)
Octakis(isothiocyanato)thorate(IV)(*4*−)

$[Th(NCS)_8]^{4\ominus}$

M 696.7 (ion)
Tetra-K salt:
$C_8K_4N_8S_8Th$ M 853.1
Colourless solid + 3.5 H_2O.
Tetra-Rb salt: [22533-64-8].
Colourless solid. + $2H_2O$. Ir $\nu_{C\equiv N}$ 2097, 2086, 2073, 2060 cm^{-1} (nujol); 2088, 2055 cm^{-1} (Me_2CO).
Tetra-Cs salt: Colourless solid + $2H_2O$. Ir $\nu_{C\equiv N}$ 2087, 2048 cm^{-1} (Me_2CO); 2092, 2083, 2062, 2055 cm^{-1}(nujol).
Tetra-NH_4 salt: Colourless solid + $2H_2O$.
Tetrakis-Et_4N salt: [38356-72-8].
White cryst. Sol. MeCN, $MeNO_2$, Me_2CO. Ir $\nu_{C\equiv N}$ 2045 cm^{-1}. 8-Coordinate cubic struct; isomorphous with U analogue.
Molodkin, A.K. *et al, Zh. Neorg. Khim.*, 1962, **7**, 1548; 1964, **9**, 60; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1962, **7**, 800; 1964, **9**, 32 (*synth, ir*)
Arutyunyan, E.G. *et al, Zh. Strukt. Khim.*, 1963, **4**, 110; *J. Struct. Chem. USSR (Engl. Transl.)*, 1963, **4**, 96.
Bagnall, K.W. *et al, J. Chem. Soc.*, 1964, 2527 (*synth*)
Grey, I.E. *et al, Aust. J. Chem.*, 1969, **22**, 311 (*synth*)
Al-Kazzaz, Z.M.S. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2273 (*synth, ir*)
Charpin, P. *et al, Acta Crystallogr., Sect. C*, 1983, **39**, 190 (*cryst struct*)

$C_8N_8S_8U^{4\ominus}$ IC-006414
Octakis(thiocyanato-*N*)uranate(*IV*)
Octakis(isothiocyanato)uranate(IV)(*4*−)

$[U(NCS)_8]^{4\ominus}$

M 702.6 (ion)
Tetra-K salt:
$C_8K_4N_8S_8U$ M 859.0
Grey-green solid.
Tetra-Rb salt: Green solid + H_2O. Ir $\nu_{C\equiv N}$ 2088, 2050 cm^{-1} (Me_2CO); 2097, 2087, 2073, 2061 cm^{-1} (nujol).
Tetra-Cs salt: [22533-67-1].
Green solid + H_2O. Ir $\nu_{C\equiv N}$ 2087, 2052 cm^{-1} (Me_2CO); 2098, 2086, 2064, 2012 cm^{-1} (nujol).
Tetra-NH_4 salt: [22533-68-2].
Grey-green solid. Ir $\nu_{C\equiv N}$ 2087, 2049 cm^{-1} (Me_2CO); 2097 2072 cm^{-1} (nujol).
Tetrakis-Et_4N salt: [33724-34-4].
Dark green solid (MeCN). Sol. MeCN. Mp 242°. Ir $\nu_{C\equiv N}$ 2095, 2060 cm^{-1} (nujol).
Markov, V.P. *et al, Zh. Neorg. Khim.*, 1961, **6**, 2316; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1961, **6**, 1175 (*synth*)
Arutyunyan, E.G. *et al, Zh. Strukt. Khim.*, 1963, **4**, 110; *J. Struct. Chem. USSR (Engl. Transl.)*, 1963, **4**, 96.
Bagnall, K.W. *et al, J. Chem. Soc.*, 1964, 2527 (*synth*)
Grey, I.E. *et al, Aust. J. Chem.*, 1969, **22**, 311.
Countryman, R. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 2213 (*cryst struct*)
Gans, P. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1738 (*synth, uv, magnetism*)
Al-Kazzaz, Z.M.S. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 2273 (*synth, ir*)
Bombieri, G. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1520 (*cryst struct*)
Folcher, G. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 743 (*magnetism*)

Soulie, E. *et al, Theor. Chim. Acta*, 1976, **41**, 7; 1979, **51**, 259 (*magnetism*)
Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 1057 (*ir, raman*)

IC-006415

$C_8N_8Ti^{5\ominus}$

Octakis(cyano-*C*)titanate(*III*)(5−), 10CI

$[Ti(CN)_8]^{5\ominus}$

M 256.0 (ion)
May be 7-coordinate, see Heptakis(cyano-*C*)titanate(*III*) (4−), IC-005849.

Penta-K salt:
$C_8K_5N_8Ti$ M 451.5
Synth. from KCN and $TiBr_3$ in liq. NH_3. Green solid. Paramagnetic, $\mu_{eff} = 1.71\mu_B$. Listed as $K_3Ti(CN)_6.2KCN$ in 8CI, but this formulation is probably incorr.

Nicholls, D. *et al, Inorg. Chim. Acta*, 1980, **41**, 233 (*synth, ir, uv-vis, magnetism, K salt*)

IC-006416

$C_8N_8W^{4\ominus}$

Octakis(cyano-*C*)tungstate(*IV*)(4−), 10CI, 9CI
Octacyanotungstate(IV), *8CI*
[18177-17-8]

$[W(CN)_8]^{4\ominus}$ (D_{2d})

M 391.9 (ion)
Dodecahedral. Undergoes photolysis. Used as anion-exchange polymer film for electrodes. Good reducing agent. Many salts known, diamagnetic.

Tetra-K salt: [17475-73-9].
Orange tetragonal cryst. (aq. EtOH). Forms a dihydrate.
Tetra-NH_4 salt: [12083-19-1].
[17457-90-8]

Inorg. Synth., 1963, **7**, 142 (*synth*)
Lippard, S.J. *et al, Inorg. Chem.*, 1967, **6**, 1943.
Hartman, K.O. *et al, Spectrochim. Acta, Part A*, 1968, **24**, 669 (*raman, ir*)
Waltz, W.L. *et al, J. Phys. Chem.*, 1969, **73**, 4250 (*mech*)
Ohsaka, T. *et al, J. Electroanal. Chem. Interfacial Electrochem.*, 1986, **200**, 159.
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 973 (*rev*)

IC-006417

$C_8N_8W^{3\ominus}$

Octakis(cyano-*C*)tungstate(*V*)(3−)
[17568-76-2]

$[W(CN)_8]^{3\ominus}$

M 391.9 (ion)
Ion is dodecahedral or square antiprismatic depending on the cation or solv.

Tri-Na salt: [29967-08-6].
Synth. from $K_4[W(CN)_8].2H_2O$, $Ce(SO_4)_2$, $AgNO_3$ and NaCl. Orange-yellow cryst. $+3H_2O$ (H_2O).
Tri-K salt: Synth. from $K_3W_2Cl_9$ and KCN. Orange-yellow cryst. $+2H_2O$ (aq. EtOH). $\mu_{eff} = 1.84\mu_B$.
Tri-Ag salt: [52239-58-4].
Synth. from $K_4[W(CN)_8].2H_2O$, $Ce(SO_4)_2$ and $AgNO_3$. Red powder.
Tris-tetrabutylammonium salt: [52239-57-3].
Synth. from $K_4[W(CN)_8].2H_2O$, $KMnO_4$, $AgNO_3$, HCl and Bu_4NBr. Colourless cryst. (MeCN/Et_2O), dec. in light.

Inorg. Synth., 1963, **7**, 142 (*synth, K salt, dihydrate*)
Bok, L.D.C. *et al, Acta Crystallogr., Sect. B*, 1970, **26**, 684 (*cryst struct, synth, Na salt, tetrahydrate*)
Pribush, R.A. *et al, Inorg. Chem.*, 1974, **13**, 2556 (*synth, esr, uv, mcd, Na, K, Ag, Bu_4N salts*)
Kiernan, P.M. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 2489 (*ir, raman, esr, Na, K, Bu_4N salt*)

IC-006418

$C_8N_{12}Zn^{2\ominus}$

Tetrakis(carbonimidoylcyanamidato)zincate(2−), 11CI
Tetrakis(dicyanamido)zincate(2−)

$[Zn(NCNCN)_4]^{2\ominus}$

M 329.5 (ion)

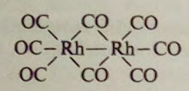
Di-K salt: [107102-28-3].
Colourless cryst. (DMSO/Et_2O). Dec. at 150°.
Bis-Ph_4P salt: [107087-49-0].
Colourless cryst. (Me_2CO). Mp 193°.
Bis-Ph_4As salt: [107102-26-1].
Colourless cryst. (Me_2CO). Mp 170°.

Köhler, H. *et al, Z. Anorg. Allg. Chem.*, 1986, **542**, 59 (*synth, ir, N-15 nmr, cmr, esca*)

IC-006419

$C_8O_8Rh_2$

Di-μ-carbonylhexacarbonyldirhodium, 10CI
Octacarbonyldirhodium, 9CI. Rhodium carbonyl, 8CI. Dirhodium octacarbonyl
[29658-60-4]



M 429.8
V. unstable. Disproportionates to $Rh_4(CO)_{12}$ at r.t. Ir ν_{CO} 2060s, 2043s, 2038s, 1852w, 1830m cm^{-1}.

Whyman, R., *J. Chem. Soc., Dalton Trans.*, 1972, 1375 (*ir*)
Hanlan, L.A. *et al, J. Am. Chem. Soc.*, 1974, **96**, 6324 (*ir*)
Hanlan, A.J.L. *et al, Inorg. Chem.*, 1979, **18**, 1790 (*uv*)
Vidal, J.L. *et al, Inorg. Chem.*, 1981, **20**, 249 (*ir*)

IC-006420

$C_8O_{16}Th^{4\ominus}$

Tetrakis(oxalato)thorate(*IV*)(4−)
Tetrakis(ethanedioato-O,O′)thorate(4−)

$[Th(C_2O_4)_4]^{4\ominus}$

M 584.1 (ion)
Obt. as ppts. with various counter ions.

Tetra-K salt: [56111-08-1].
Colourless plates $+ 4H_2O$. Partly sol. H_2O with loss of oxalate. 10-Coordinate bicapped square antiprismatic at Th.
Tetra-NH_4 salt: [21293-75-4].
Colourless cryst. $+ 3H_2O$. Sol. H_2O.

[12083-31-7, 21029-51-6]

Berzelius, J., *Pogg. Ann.*, 1829, **16**, 385 (*synth*)
Inorg. Synth., 1966, **8**, 43 (*synth*)
Molodkhin, A.K. *et al, Zh. Neorg. Khim.*, 1968, **13**, 2117; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1095 (*synth*)
Kharitonov, Y.Y. *et al, Zh. Neorg. Khim.*, 1968, **13**, 2315; 1973, **18**, 2869; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 1196; 1973, **18**, 1524 (*ir*)
Petrzhak, G.I. *et al, Radiokhimiya*, 1974, **16**, 200 (*ir*)

Nefedov, V. *et al, Zh. Neorg. Khim.*, 1974, **19**, 2628; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 1435 (*pe*)
Akhter, M.M. *et al, Acta Chem. Scand., Ser. B*, 1975, **31**, 1361 (*cryst struct*)
Hoshi, M. *et al, Radiochem. Radioanal. Lett.*, 1977, **29**, 331 (*synth*)

IC-006421

$C_8O_{16}U^{4\ominus}$

Tetrakis(oxalato)uranate(*IV*)(4−)
Tetrakis(ethanedioato-O,O′)uranate(4−)

$[U(C_2O_4)_4]^{4\ominus}$

M 590.1 (ion)
Pptd. by many cations.

Tetra-Na salt: [101196-72-9].
Green solid $+ 1H_2O$. On heating forms sodium uranate(*VI*).
Tetra-K salt: [21135-81-9].
Light green cryst. $+ 5H_2O$, or grey-green solid. Sol. H_2O. $\mu_{eff} = 3.62\mu_B$ ($2.94\mu_B$). Loses H_2O at 185° to form anhyd. salt. Also obt. as octahydrate. Dec. to K_2UO_4 at 900°.
Tetra-Cs salt: [52880-38-3].
V. hygroscopic green solid $+ 3H_2O$.
Di-Ba salt: [55336-49-7].
Cryst. $+ 8H_2O$. Less sol. than K salt. Similar compds. obtd. with other Gp II metals. $\mu_{eff} = 3.60\ \mu_B$ (θ 135°). 9-Coordinate U in tricapped trigonal prismatic environment of 4 bidentate oxalate ligands and one H_2O.
Tetra-NH_4 salt: [52880-37-2].
Dark green solid $+ 6H_2O$. Paramagnetic; $\mu_{eff} = 2.53\mu_B$ (293K).

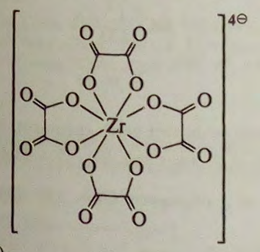
[53457-55-9]

Inorg. Synth., 1950, **3**, 169; 1966, **8**, 157.
Awasthi, S.K. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 3805; 1974, **36**, 2521 (*synth, tga, ir, magnetism*)
Petrzhak, G.I. *et al, Radiokhimiya*, 1974, **16**, 200 (*ir*)
Brown, D. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1853 (*use*)
Spirlet, M.R. *et al, J. Less-Common Met.*, 1986, **122**, 205 (*cryst struct*)

IC-006422

$C_8O_{16}Zr^{4\ominus}$

Tetrakis(oxalato)zirconate(*IV*)(4−)
Tetrakis[ethanedioato(2−)-O,O′]zirconate(IV)(4−), *11CI*
[21392-82-5]



M 443.3 (ion)
8-Coord. dodecahedral at Zr. Synth. from $ZrOCl_2.8H_2O$ and an appropriate oxalate in H_2O followed by precipitation with EtOH. The salts act as cytochrome-C inhibitors. The potassium and ammonium salts are used in the synthesis of olefin polym. catalyst supports and in analysis of zirconium. Degree of hydration variable. Sol. H_2O.

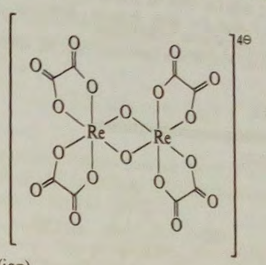
Tetra-Na salt, trihydrate: [77171-21-2].
White solid (EtOH aq.).
Tetra-K salt: [12083-35-1].
White solid (EtOH aq.).
Tetra-K salt, pentahydrate: [67375-34-2].
White solid.
Tetra-NH_4 salt: [77122-59-9].
White solid.

Glen, G.L. *et al, Inorg. Chem.*, 1963, **2**, 250 (*cryst struct, Na_4 salt, synth*)
Inorg. Synth., 1966, **8**, 40; 1968, **11**, 53 (*synth*)
Kojic-Prodic, B. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 2001 (*cryst struct, $K_4.5H_2O$ salt*)
U.S. Pat., 4 279 780, (1981); *CA*, **95**, 151462q (*use*)
Ishimori, T. *et al, Talanta*, 1984, **31**, 621 (*anal*)
Beoku-Betts, D. *et al, Inorg. Chem.*, 1985, **24**, 1142,1677 (*pharmacol*)

IC-006423

$C_8O_{18}Re_2^{4\ominus}$

Tetrakis(oxalato)di-μ-oxodirhenate(*IV*)(4−)
Tetrakis[ethanedioato(2−)-O,O-o]di-μ-oxodirhenate(IV)(4−), *9CI*



M 756.4 (ion)
Re—Re distance: 236.2 pm.

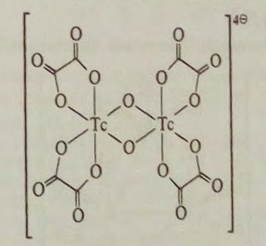
Tetra-K salt: [56349-59-8].
Synth. from ReO_2, oxalic acid and K oxalate under reflux. Green-red cryst. $+ 3H_2O$ (H_2O).

Lys, T., *Acta Crystallogr., Sect. B*, 1975, **31**, 1594 (*synth, cryst struct*)

IC-006424

$C_8O_{18}Tc_2^{4\ominus}$

Tetrakis(oxalato)-di-μ-oxoditechnetate(*IV*)(4−)



M 581.8 (ion)
Strong Tc—Tc interaction. Synth. from K_2TcF_6 + $K_2(C_2O_4)$ in water (80° for 3 d). Stable and inert in aq. media.

Tetra-K salt: [133982-84-0].
Dark red triclinic cryst. $+ 3H_2O$ (EtOH aq.). Insol. EtOH.

Alberto, R. *et al, Inorg. Chim. Acta*, 1990, **178**, 125 (*synth, cryst struct, uv, ir*)

IC-006425

C_8Rb

Rubidium graphite (RbC_8), 9CI

Graphite compd. with rubidium (8:1), 10CI. Rubidium-graphite intercalate. Rubidium-graphite lamellar compd.

[12193-29-2]

C_8Rb

M 181.5

Member of a family of compds. of differing stoichiometries (C_8Rb, $C_{12}Rb$, $C_{24}Rb$ etc.). Orthorhombic. The graphite struct. is retained with Rb atoms stacked vertically between planes. The unit cells are twisted (120°) with respect to each other. Synth. by direct action of graphite with Rb vapour at 300°. Hydrogenation catalyst. Moisture-sensitive shiny black powder.

▷ Reacts violently with H_2O to form graphite and RbOH.

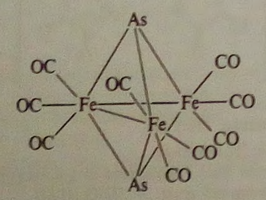
Lagrange, P. *et al, Proc. London Int. Carbon, Graphite Conf., 5th,* 1978, **2**, 660; *CA*, 1980, **92**, 224646 (*cryst struct*)
Lauginie, P. *et al, Ext. Abstr. Program - Bienn Conf. Carbon*, 1979, **14**, 312 (*cmr;OCA*, **91**, 219832 (*cmr*)
Solin, S.A. *et al, J. Raman Spectrosc.*, 1981, **10**, 129 (*raman*)

IC-006426

$C_9As_2Fe_3O_9$

Di-μ_3-arsenidononacarbonyltriiron

[40742-82-3]



M 569.4

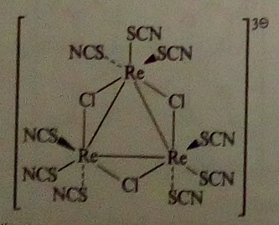
Violet-black cryst. (pet. ether). Mp >150° dec. $Subl._{0.05}$ 105°.

Delbaere, L.T.J. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 307 (*synth, struct, ms, ir*)

IC-006427

$C_9Cl_3N_9Re_3S_9^{3\ominus}$

Tri-μ-chlorononakis(thiocyanato-*S*)trirhenate(*III*)(3−)



M 1187.7 (ion)

Tris-Ph₃MeAs salt: Synth. from Re_3Cl_9, $Ph_3MeAsBr$ and HCNS aq. Dark brown-green powder.

Robinson, B.H. *et al, J. Chem. Soc.*, 1964, 5683 (*synth, uv, props*)

IC-006428

$C_9CoCrO_9^{\ominus}$

Nonacarbonylcobaltatechromate(1−), 8CI

Pentacarbonyl(tetracarbonylcobalt)chromate(1−)

$[(OC)_4Co—Cr(CO)_5]^{\ominus}$

M 363.0 (ion)

Bis(triphenylphosphine)iminium salt: Orange, mod. air-stable cryst. (Et_2O/pentane). Soln. unstable. Sol. Et_2O, THF. Mp 73-75° dec. Ir ν_{CO} 2055w, 2000w, 1936vs, 1910w, 1864m, 1854m cm^{-1} (nujol).

Ruff, J.K., *Inorg. Chem.*, 1968, **7**, 1818 (*synth, ir*)

IC-006429

C_9CoMnO_9

Pentacarbonyl(tetracarbonylcobalt)manganese, 10CI, 9CI

Nonacarbonylcobaltmanganese

[35646-82-3]

$(OC)_4Co—Mn(CO)_5$

M 365.9

Synth. from $[Mn(CO)_6][Co(CO)_4]$ at 20° in THF. Red-brown cryst., air-sensitive in soln. V. sol. most org. solvs. Mp 46°. $Subl._{0.1}$ 30°. Ir ν_{CO} 2117w, 2058s, 2025s, 1994m, 1981sh cm^{-1} (CCl_4).

Joshi, K.K. *et al, Z. Naturforsch., B*, 1962, **17**, 565 (*synth, ir*)
Kruck, T. *et al, Chem. Ber.*, 1964, **97**, 2289 (*synth, ir*)
Mooberry, E.S. *et al, J. Chem. Phys.*, 1972, **56**, 1852 (*Co-59 nmr*)
Madach, T. *et al, Chem. Ber.*, 1980, **113**, 2675 (*synth, props*)
Sbrignadello, G., *Inorg. Chim. Acta*, 1981, **48**, 237 (*ir*)

IC-006430

$C_9CoO_9W^{\ominus}$

Nonacarbonylcobaltatetungstate(1−), 8CI

Pentacarbonyl(tetracarbonylcobaltate)tungstate(1−)

$[(OC)_4Co—W(CO)_5]^{\ominus}$

M 494.8 (ion)

Bis(triphenylphosphine)iminium salt: Orange, mod. air-stable cryst. (Et_2O/pentane). Unstable in soln. Sol. Et_2O, THF. Mp 111-113° dec. Ir ν_{CO} 2062w, 2012m, 1940vs, 1912w, 1864m cm^{-1} (nujol).

Ruff, J.K., *Inorg. Chem.*, 1968, **7**, 1818 (*synth*)

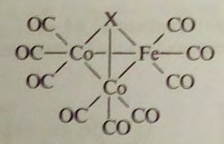
IC-006431

$C_9Co_2FeO_9Se$

Tricarbonyl(hexacarbonyldicobalt)-μ_3-selenoxoiron, 9CI

Nonacarbonyl-μ_3-selenoxodicobaltiron

[35163-36-1]



X = Se

M 504.7

Air-stable black or brown cryst. (pentane). Mp 104-106°.

Strouse, C.E. *et al, J. Am. Chem. Soc.*, 1971, **93**, 6032 (*synth, struct, ir*)
Seyferth, D. *et al, J. Organomet. Chem.*, 1981, **204**, 333 (*synth, ir, ms*)

IC-006432

$C_9Co_2FeO_9Te$

Tricarbonyl(hexacarbonyldicobalt)-μ_3-telluroxoiron

Nonacarbonyl-μ_3-telluroxoiron

[35163-37-2]

As Tricarbonyl(hexacarbonyldicobalt)-μ_3-selenoxoiron with

X = Te

M 553.4

Brown cryst. (hexane).

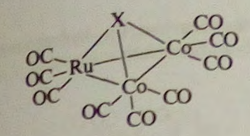
Strouse, C.E. *et al, J. Am. Chem. Soc.*, 1971, **93**, 6032 (*synth, ir, struct*)

IC-006433

$C_9Co_2O_9RuS$

Tricarbonyl(hexacarbonyldicobalt)-μ_3-thioxoruthenium, 11CI

[86272-87-9]



X = S

M 503.0

Black cryst. (hexane). Mp 120°.

Roland, E. *et al, Chem. Ber.*, 1984, **117**, 1039 (*synth, ir*)

IC-006434

$C_9Co_2O_9RuSe$

Tricarbonyl(hexacarbonyldicobalt)-μ_3-selenoxoruthenium, 11CI

[86272-88-0]

As Tricarbonyl(hexacarbonyldicobalt)-μ_3-thioxoruthenium, IC-006433 with

X = Se

M 549.9

No phys. props. descr.

Roland, E. *et al, Organometallics*, 1983, **2**, 1048 (*synth, ir*)

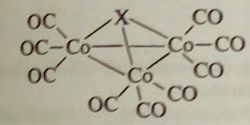
IC-006435

$C_9Co_3O_9S$

Nonacarbonyl-μ_3-thioxotricobalt, 10CI

Tricobalt enneacarbonyl sulfide

[35260-81-2]



X = S

M 460.9

Black or dark-brown air-sensitive cryst. (hexane). Ir ν_{CO} 2103w, 2050vs, 2038m, 2024w cm^{-1} (heptane). Paramagnetic.

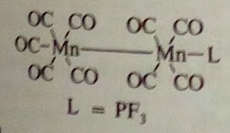
Markó, L. *et al, Chem. Ber.*, 1963, **96**, 955 (*synth, ir*)
Wei, C.H. *et al, Inorg. Chem.*, 1967, **6**, 1229 (*synth, cryst struct*)
Oxton, I.A. *et al, Inorg. Chim. Acta*, 1981, **47**, 177 (*ir*)

IC-006436

$C_9F_3Mn_2O_9P$

Nonacarbonyl(phosphorous trifluoride)dimanganese, 9CI

Nonacarbonyl(trifluorophosphine)dimanganese



axial-form

L = PF_3

M 449.9

Synth. from $Mn_2(CO)_{10}$ and PF_3. Yellow solid, sensitive to hydroxylic solvs. Mp 90°. Ir ν_{CO} 2110, 2038, 2015, 2002, 1992, 1980, 1960, 1954 cm^{-1} (hexane). Subl. *in vacuo*.

Clark, R.J. *et al, Inorg. Chem.*, 1968, **7**, 673 (*synth, ir*)

IC-006437

$C_9F_3O_9PTc_2$

Nonacarbonyl(phosphorus trifluoride)ditechnetium, 12CI

[125996-69-2]

$(OC)_5Tc—Tc(CO)_4(PF_3)$

M 537.8

PF_3 is axial. Synth. by thermal or photochemical reaction of $Tc_2(CO)_{10}$ with PF_3. Further reaction with more PF_3 gives $Tc_2(CO)_8(PF_3)_2$, $Tc_2(CO)_7(PF_3)_3$, $Tc_2(CO)_6(PF_3)_4$, etc., up to $Tc_2(CO)_2(PF_3)_8$. 24 Tc—CO—PF_3 species are known.

[125996-63-6, 125996-66-9, 125996-68-1, 126061-08-3, 126061-10-7, 126061-11-8, 126061-12-9]

Grimm, C.C. *et al, Inorg. Chim. Acta*, 1989, **159**, 137 (*F-19 nmr, Tc-99 nmr*)
Grimm, C.C. *et al, Organometallics*, 1990, **9**, 1123 (*gc, analogues*)

IC-006438

$C_9FeMnO_9^{\ominus}$

Nonacarbonylferratemanganate(1−), 8CI

Pentacarbonyl(tetracarbonylferrate)manganate(1−)

[84143-94-2]

$[(OC)_5Mn—Fe(CO)_4]^{\ominus}$

M 362.8 (ion)

Bis(triphenylphosphine)iminium salt: Synth. from $Fe(CO)_5$ and $[(Ph_3P)_2N]Mn(CO)_5$ in THF. Dark-red cryst. (pentane/Et_2O). Mp 134-135°.

Ruff, J.K., *Inorg. Chem.*, 1968, **7**, 1818 (*synth, ir*)
Ozin, G.A. *et al, Organometallics*, 1983, **2**, 415 (*synth, ir*)

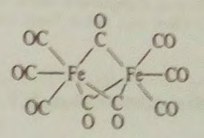
IC-006439

$C_9Fe_2O_9$

Tri-μ-carbonylhexacarbonyldiiron, 9CI

Nonacarbonyldiiron. Diiron enneacarbonyl. Iron carbonyl ($Fe_2(CO)_9$)

[15321-51-4]



M 363.7

Has various synthetic applications. Orange hexagonal leaflets. Insol. org. solvs. Mp 100-120° dec. (80° dec.).

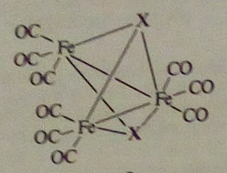
Inorg. Synth., 1966, **8**, 178 (*synth*)
U.K. Pat., 1 130 676, (1968); *CA*, **70**, 33233 (*synth*)
Griffith, W.P. *et al, J. Chem. Soc. A*, 1969, 834 (*ir, raman*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 1827 (*synth*)
Cotton, F.A., *Prog. Inorg. Chem.*, 1976, **21**, 1 (*rev, struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 498 (*uses*)
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 670.
Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 421.

IC-006440

$C_9Fe_3O_9S_2$

Nonacarbonyldi-μ_3-thioxotriiron, 9CI, 8CI

[22309-04-2]



X = S

M 483.7

Ruby-red or black-red cryst. (toluene/pentane). Mp 114°.

Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **296**, 91 (*synth, ir*)
Wei, C.H. *et al*, *Inorg. Chem.*, 1965, **4**, 493 (*struct*)
Chaudhuri, M.K. *et al*, *J. Organomet. Chem.*, 1977, **124**, 37 (*ms*)
Nametkin, N.S. *et al*, *J. Organomet. Chem.*, 1978, **149**, 355.
Aime, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 46 (*cmr*)
Huebener, P. *et al*, *Cryst. Struct. Commun.*, 1982, **11**, 331 (*cryst struct*)
Rives, A.B. *et al*, *Inorg. Chem.*, 1982, **21**, 2286 (*struct*)
Winter, A. *et al*, *J. Organomet. Chem.*, 1982, **234**, 337 (*synth, ir, ms*)

IC-006441

$C_9Fe_3O_9Se_2$

Nonacarbonyldi-μ_3-selenoxotriiron, 9CI, 8CI

[22587-69-5]

As Nonacarbonyldi-μ_3-thioxotriiron, IC-006440 with

X = Se

M 577.5

Dark-violet needles (pet. ether).

Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **296**, 91 (*synth, ir*)
Dahl, L.F. *et al*, *Inorg. Chem.*, 1963, **2**, 1067 (*struct*)
Cetini, G. *et al*, *J. Organomet. Chem.*, 1968, **15**, 373.
Chaudhuri, M.K. *et al*, *J. Organomet. Chem.*, 1977, **124**, 37 (*ms*)
Aime, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 46 (*cmr*)

IC-006442

$C_9Fe_3O_9Te_2$

Nonacarbonyldi-μ_3-telluroxotriiron, 8CI

[22587-70-8]

As Nonacarbonyldi-μ_3-thioxotriiron, IC-006440 with

X = Te

M 674.8

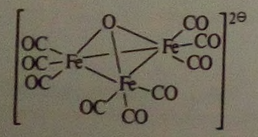
Fine black-green cryst. (CH_2Cl_2/MeOH).

Hieber, W. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **296**, 91 (*synth, ir*)
Chaudhuri, M.K. *et al*, *J. Organomet. Chem.*, 1977, **124**, 37 (*ms*)
Aime, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 46 (*cmr*)
Lesch, D.A. *et al*, *Inorg. Chem.*, 1981, **20**, 3583 (*synth, nmr, ms*)
Lesch, D.A. *et al*, *Organometallics*, 1982, **1**, 499 (*ir, props*)

IC-006443

$C_9Fe_3O_{10}^{2\ominus}$

Nonacarbonyl-μ_3-oxotriferrate(2−), 11CI



M 435.6 (ion)

Bis(benzyltrimethylammonium) salt: [86465-89-6].

Red-orange cryst. (THF/cyclohexane).

Ceriotti, A. *et al*, *J. Organomet. Chem.*, 1983, **249**, C35 (*synth, struct, ir*)

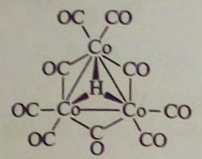
IC-006444

$C_9HCo_3O_9$

Tri-μ-carbonylhexacarbonyl-μ_3-hydrotricobalt, 10CI

Nonacarbonylhydridotricobalt

[71204-90-5]



M 429.9

Blackish-green cryst. (hexane/toluene). Thermally unstable giving $Co_4(CO)_{12}$ above 30°.

Fachinetti, G. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1979, **18**, 619; 1981, **20**, 204 (*synth, ir, ms, cryst struct*)

IC-006445

$C_9HFeO_9W^{\ominus}$

Pentacarbonyl-μ-hydro(tetracarbonylferrate) tungstate(1−), 11CI

$[(OC)_5W{-}H{-}Fe(CO)_4]^{\ominus}$

M 492.7 (ion)

Bis(triphenylphosphine)iminium salt: [88326-15-2]. Yellow-orange solid (MeOH/hexane), stable in air for short periods. Sol. MeOH.

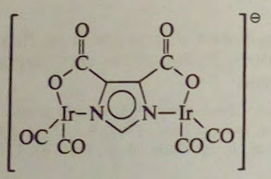
Arndt, L. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 456 (*synth, ir, nmr, cryst struct*)

IC-006446

$C_9HIr_2N_2O_8^{\ominus}$

Tetracarbonyl[μ-[1*H*-imidazole-4,5-dicarboxylato(3−)-$N^3,O^5{:}N^3,O^4$]]diiridate(1−)

[μ-Imidazole-4,5-dicarboxylato(3−)]bis[dicarbonyliridate] (1−)



M 649.5 (ion)

Exhibits strong colours due to intermol. stacking interactions, which are modulated by counter cation. Semiconductor.

K salt: [116746-30-6].
$C_9HIr_2KN_2O_8$ M 688.6
Dark-blue solid + $2H_2O$. Insol. Ir ν_{CO} 2075m,br, 1995s,br cm^{-1} (nujol).

Me_4N salt: [116746-12-4].
$C_{13}H_{17}Ir_2N_3O_{10}$ M 759.7
Solid + $2H_2O$. Insol. λ_{max} 760 nm (nujol).

Et_4N salt: [116746-13-5].
$C_{17}H_{27}Ir_2N_3O_{11}$ M 833.8
Solid + $3H_2O$. Insol. λ_{max} 620 nm (nujol).

Tetrabutylammonium salt:
$C_{25}H_{37}Ir_2N_3O_8$ M 892.0

Solid. V. sol. CH_2Cl_2, MeCN. λ_{max} 435 sh (ε 380), 395 sh (ε 650), 355 sh (ε 1470) nm (MeCN).

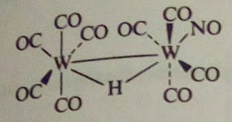
Bayón, J.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 3003 (*synth, ir, uv, props*)

IC-006447

$C_9HNO_{10}W_2$

Nonacarbonyl-μ-hydronitrosylditungsten, 9CI

[40270-21-1]



M 650.8

NO group axial, bent staggered struct. Orange cryst. (CH_2Cl_2). Sol. common org. solvs. Mp 128-129.5°. Air-stable as solid but mod. air-sensitive in soln.

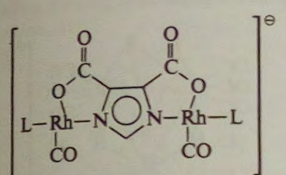
King, R.B. *et al*, *Inorg. Chem.*, 1974, **13**, 3038 (*props*)
Bau, R. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 6621 (*synth, cryst struct*)
Angelici, R.J. *et al*, *Inorg. Chem.*, 1976, **15**, 2397 (*synth*)

IC-006448

$C_9HN_2O_8Rh_2^{\ominus}$

Tetracarbonyl[μ-[1*H*-imidazole-4,5-dicarboxylato(3−)-$N^3,O^5{:}N^3,O^4$]]dirhodate(1−)

μ-Imidazole-4,5-dicarboxylato(3−)bis[dicarbonylrhodate] (1−)



L = CO

M 470.9 (ion)

Exhibits strong colours due to intermol. stacking interactions, modulated by counter cation. Semiconductor.

Me_4N salt: [116746-08-8].
$C_{13}H_{18}N_3O_9Rh_2$ M 563.0
Mod. air-stable dichroic cryst. + $1H_2O$. Air-sensitive in soln. Ir ν_{CO} 2090s, 2080s, 2025s, 2010s cm^{-1} (nujol); λ_{max} 650 nm (nujol).

Et_3NH salt: [116746-06-6].
$C_{15}H_{17}N_3O_8Rh_2$ M 573.1
Mod. air-stable dichroic cryst., air-sensitive in soln. Ir ν_{CO} 2095, 2070, 2040, 2015 cm^{-1} (nujol).

Et_4N salt: [116746-09-9].
$C_{17}H_{21}N_3O_8Rh_2$ M 601.1
Mod. air-stable dichroic cryst., air-sensitive in soln. Ir ν_{CO} 2090s,br, 2030s, 2010 cm^{-1} (nujol), λ_{max} 520 nm (nujol).

Tetrabutylammonium salt, monohydrate: [116746-10-2].
$C_{28}H_{39}N_3O_9Rh_2$ M 731.4
Mod. air-stable cryst. (Et_2O), air-sensitive in soln. V. sol. CH_2Cl_2, MeCN. Ir ν_{CO} 2085, 2020 cm^{-1} (CH_2Cl_2). λ_{max} 430(ε 320), 340 (ε 3 300) nm (MeCN).

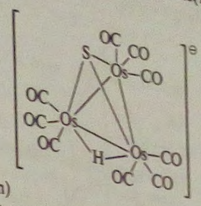
Bayón, J.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 3003 (*synth, ir, uv, props*)

IC-006449

$C_9HO_9Os_3S^{\ominus}$

Nonacarbonyl-μ-hydro-μ_3-thioxotriosmate(1−)

[68796-19-0]



M 855.7 (ion)

Bis(triphenylphosphine)iminium salt: [69085-99-0]. Yellow.

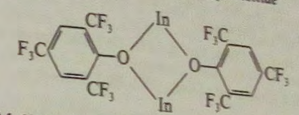
Johnson, B.F.G. *et al*, *Acta Crystallogr., Sect. B*, 1978, **34**, 3767 (*cryst struct*)
Johnson, B.F.G. *et al*, *J. Organomet. Chem.*, 1981, **213**, 249 (*synth, ir, pmr*)

IC-006450

$C_9H_2F_9InO$

[2,4,6-Tris(trifluoromethyl)phenolato]indium(*I*)

Indium 2,4,6-tris(trifluoromethyl)phenoxide



Dimer

M 411.9

Dimeric.

Dimer: Bis[μ-[2,4,6-tris(trifluoromethyl)phenolato]]diindium $C_{18}H_4F_{18}In_2O_2$ M 823.8
From $(CF_3)_3C_6H_2OH$ + $(C_5H_5)_3In$ in hexane. White air- and moisture-sensitive solid (hexane).

Scholz, M. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1989, **28**, 1383 (*synth, ir, pmr, F-19 nmr, cryst struct*)

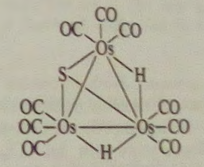
IC-006451

$C_9H_2O_9Os_3S$

Nonacarbonyldi-μ-hydro-μ_3-thioxotriosmium

1,1,1,2,2,2,3,3,3-Nonacarbonyl-1,2;1,3-di-μ-hydrido-μ_3-sulfidotriosmium

[38979-82-7]



M 856.7

Pale-yellow cryst.

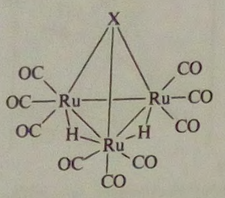
Forster, A. *et al*, *J. Organomet. Chem.*, 1976, **104**, 225 (*pmr, cmr*)
Johnson, B.F.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 616 (*struct*)
Adams, R.D. *et al*, *Organometallics*, 1984, **3**, 548 (*synth*)

$C_9H_2O_9Ru_3S$ IC-006452

Nonacarbonyldi-μ-hydro-μ_3-thioxotriruthenium, 9CI

Nonacarbonyldihydridosulfidotriruthenium

[11127-38-1]



X = S

M 589.3

An unconfirmed report suggests the complex is paramagnetic (surprisingly), early ir data is suspect. Synth. by treating $Ru_3(CO)_{12}$ in boiling heptane with H_2S, or $Ru_3(CO)_{12}$ in boiling octane with elemental sulfur under CO/H_2 (35 atm), or Nonacarbonyltri-μ-hydro-μ_3-thioxotriruthenium(1+), IC-006456 with H_2O. Air-sensitive yellow cryst. (C_6H_6). Sol. hexane, CCl_4. Mp 118°. Ir ν_{CO} 2118, 2085, 2061, 2050, 2020, 2011, 2000, 1995, 1968 cm^{-1} (hexane).

Deeming, A.J. *et al, J. Chem. Soc. A*, 1971, 1797, 2701 (*synth, ir, pmr, ms*)
Sappa, E. *et al, J. Organomet. Chem.*, 1972, **35**, 375 (*synth, ir, magnetism*)
Forster, A. *et al, J. Organomet. Chem.*, 1976, **104**, 225 (*cmr*)
Johnson, B.F.G. *et al, J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir, pmr, ms*)
Johnson, B.F.G. *et al, J. Organomet. Chem.*, 1980, **190**, C91 (*reactions*)
Cresswell, T.A. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 2220 (*synth*)
Adams, R.D. *et al, Organometallics*, 1982, **1**, 53 (*synth, bibl, cryst struct*)

$C_9H_2O_9Ru_3Se$ IC-006453

Nonacarbonyldi-μ-hydro-μ_3-selenoxotriruthenium, 9CI

Nonacarbonyldihydridoselenidotriruthenium

[72268-07-6]

As Nonacarbonyldi-μ-hydro-μ_3-thioxotriruthenium, IC-006452 with

X = Se

M 636.2

Earlier ir data is suspect. Synth. by treating $Ru_3(CO)_{12}$ in boiling octane with elemental selenium under CO/H_2 (35 atm), or treating $Ru_3(CO)_{12}$ in methanolic KOH with SeO_2. Orange-yellow cryst. Sol. CCl_4. Mp 110° dec. Ir ν_{CO} 2115, 2082, 2058, 2045, 2015, 2007, 1995, 1989 cm^{-1}.

Sappa, E. *et al, J. Organomet. Chem.*, 1972, **35**, 375 (*synth, ir, pmr, ms*)
Johnson, B.F.G. *et al, J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir, pmr, ms*)

$C_9H_2O_9Ru_3Te$ IC-006454

Nonacarbonyldi-μ-hydro-μ_3-telluroxotriruthenium, 9CI

Nonacarbonyldihydridotelluridotriruthenium

[72268-08-7]

As Nonacarbonyldi-μ-hydro-μ_3-thioxotriruthenium, IC-006452 with

X = Te

M 684.9

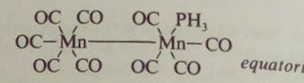
Earlier ir data is suspect. Synth. by treating $Ru_3(CO)_{12}$ in boiling octane with elemental tellurium under CO/H_2 (35 atm), or treating $Ru_3(CO)_{12}$ in methanolic KOH with TeO_2. Yellow cryst. Sol. CCl_4. Mp 135° dec. Ir ν_{CO} 2111, 2078, 2054, 2043, 2012, 2006, 1993, 1987 cm^{-1}.

Sappa, E. *et al, J. Organomet. Chem.*, 1972, **35**, 375 (*synth, ir, pmr, ms*)
Johnson, B.F.G. *et al, J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir, pmr, ms*)

$C_9H_3Mn_2O_9P$ IC-006455

Nonacarbonyl(phosphine)dimanganese, 9CI

[36329-56-3]



equatorial-form

M 395.9

Orange-yellow plates. Mp 113° dec. Ir ν_{CO} 2094w, 2023s, 2012s, 1996vs, 1970m, 1955m cm^{-1} (hexane). Subl. *in vacuo*.

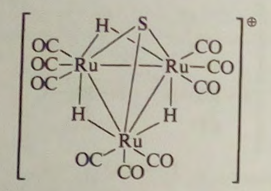
Fischer, E.O. *et al, Chem. Ber.*, 1972, **105**, 286 (*synth, ir, ms, pmr*)

$C_9H_3O_9Ru_3S^{\oplus}$ IC-006456

Nonacarbonyltri-μ-hydro-μ_3-thioxotriruthenium(1+)

Nonacarbonyltrihydridosulfidotriruthenium(1+)

[32591-91-6]



M 590.3 (ion)

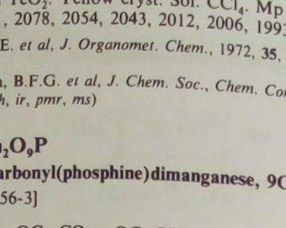
No salts isol. in the solid state. Synth. by treating Decacarbonyl[μ-(ethanethiolato)]-μ-hydrotriruthenium, IC-007427 with 98% H_2SO_4 at 100°. Yellow soln. in conc. H_2SO_4. Sol. 98% H_2SO_4. Ir ν_{CO} 2132, 2089 cm^{-1} (H_2SO_4).

Deeming, A.J. *et al, J. Chem. Soc. A*, 1971, 1797, 2701 (*synth, ir, pmr*)

$C_9H_4BFe_3O_9^{\ominus}$ IC-006457

(Borane)nonacarbonyl-μ-hydrotriferrate(1−), 11CI

[101810-38-2]



M 434.4 (ion)

Fluxional in soln.

Ph_4As salt: [101810-39-3].
Red-orange cryst. Sol. CH_2Cl_2, toluene.

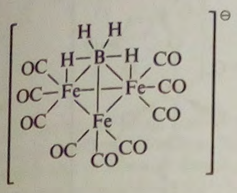
[92055-45-3]

Vites, J. *et al, Organometallics*, 1984, **3**, 1591 (*synth*)
Housecroft, C.E. *et al, Inorg. Chem.*, 1986, **25**, 404 (*reactions*)
Vites, J. *et al, J. Am. Chem. Soc.*, 1986, **108**, 3304 (*synth, ir, pmr, B-11 nmr*)
Lyman, M.M. *et al, Organometallics*, 1987, **6**, 2405 (*electronic struct*)

$C_9H_4BFe_3O_9^{\ominus}$ IC-006458

Nonacarbonyl[μ_3-[tetrahydroborato(1−)-*H*:*H*′:*H*″]]triferrate(1−)

[92055-46-4]



M 434.4 (ion)

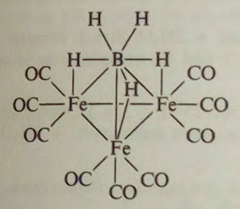
Synth. from reaction of $Na[Fe(CO)_4Ac]$ in THF with BH_3.THF and $Fe(CO)_5$ at 70° for 1 hr. No phys. props. reported.

Fehlner, T.P. *et al, Organometallics*, 1984, **3**, 1591 (*synth*)
Fehlner, T.P. *et al, Inorg. Chem.*, 1986, **25**, 404 (*reactions*)

$C_9H_5BFe_3O_9$ IC-006459

Nonacarbonyl-μ-hydro[μ_3-[tetrahydroborato(1−)-*H*:*H*′:*H*″]]triiron, 11CI

[91128-40-4]



M 435.4

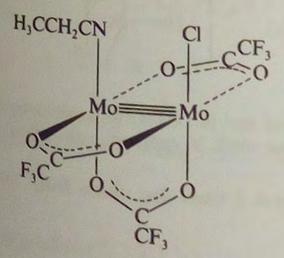
Fluxional in soln. Mod. air-stable orange cryst. (hexane). Sol. hexane, C_6H_6, toluene.

[64867-63-6, 92055-43-1]

Vites, J. *et al, J. Am. Chem. Soc.*, 1984, **106**, 4633; 1986, **108**, 3304 (*synth, cryst struct, uv, ir, pmr, B-11 nmr, ms, mössbauer*)
Lyman, M.M. *et al, Organometallics*, 1987, **6**, 2405 (*electronic struct*)

$C_9H_4ClF_9Mo_2NO_6$ IC-006460

Chloro(propanenitrile)tris[μ-(trifluoroacetato-*O*:*O*′)]dimolybdenum(*II*), 11CI



M 621.4

Mo—Mo 213.4 pm. Formed as cocrystallite (1:1) with Dichlorobis(propanenitrile)bis[μ-(trifluoroacetato-*O*:*O*′)]dimolybdenum(*II*), IC-006792. Obt. from reaction between $Mo_2(OOCCF_3)_4$, Me_3SiCl and propanenitrile in toluene at −78° to 0°. Orange cryst.

[89659-47-2]

Agaskar, P. *et al, Inorg. Chim. Acta*, 1984, **83**, 33 (*synth, cryst struct*)

$C_9H_5MnO_3S$ IC-006461

Tricarbonyl(phenylthio)manganese

(Benzenethiolato)tricarbonylmanganese

As Tricarbonyl(methanethiolato)manganese, IC-003915 with

R = Ph

M 248.1

Tetrameric. Synth. from $HMn(CO)_5$ and PhSH.

Tetramer: [24819-02-1]. *Tetrakis(μ_3-benzenethiolato)dodecacarbonyltetramanganese*
$C_{36}H_{20}Mn_4O_{12}S_4$ M 992.5
Yellow or orange cryst. (pentane). Mp 228°. Ir ν_{CO} 2028vs, 2020w,sh, 1954s cm^{-1} (cyclohexane).

Osborne, A.G. *et al, J. Chem. Soc. A*, 1966, 1143 (*synth, ir*)
Ahmad, M. *et al, J. Chem. Soc., Chem. Commun.*, 1967, 138 (*synth, ms*)
Jenkins, C.R., *J. Organomet. Chem.*, 1968, **15**, 441 (*synth, ir*)

$C_9H_5MnO_3Se$ IC-006462

Tricarbonyl(phenylseleno)manganese

(Benzeneselenolato)tricarbonylmanganese

As Tricarbonyl(methaneselenolato)manganese, IC-003916 with

R = Ph

M 295.0

Tetrameric. Synth. by heating $[Mn(SPh)(CO)_4]_2$ in cyclohexane.

Tetramer: [12304-23-3]. *Tetrakis(μ_3-benzeneselenolato)dodecacarbonyltetramanganese*
$C_{36}H_{20}Mn_4O_{12}Se_4$ M 1180.1
Orange-brown cryst. (C_6H_6). Mp 185° dec. Ir ν_{CO} 2020vs, 2013vw, 1948m cm^{-1} (cyclohexane).

Abel, E.W. *et al, J. Chem. Soc. A*, 1967, 2014 (*synth, ir*)
Jenkins, C.R., *J. Organomet. Chem.*, 1968, **15**, 441 (*synth, ir*)

$C_9H_5N_2O_9Ru^{\ominus}$ IC-006463

(Nitrosyl)bis(oxalato)(pyridine)ruthenate(1−)

Bis(ethanedioato-O,O′)(nitrosyl)(pyridine)ruthenate(1−)

$[Ru(NO)(C_2O_4)_2(Py)]^{\ominus}$

M 386.2 (ion)

Isomeric form unknown.

K salt: Prepd. by treating the K salt of Chloro(nitrosyl)bis(oxalato)ruthenate(2−), IC-003830 with Py. Red cryst.

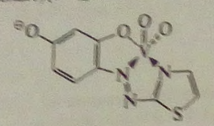
NH_4 salt: Red cryst.

Charonnat, R., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1924, **178**, 1423 (*synth*)
Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 196 (*synth*)

$C_9H_5N_3O_4SV^{\ominus}$ IC-006464

Dioxo[4-(2-thiazolylazo)-1,3-benzenediolato(2−)]vanadate(*V*)(1−), 10Cl

Dioxo[4-(1,3-thiazol-2-ylazo)resorcinolato]vanadate(V)(1−). [2-Hydroxy-2,5-cyclohexadiene-1,4-dione-1-(2-thiazolylhydrazonato)(2−)]dioxovanadate(V)(1−), 11Cl



M 302.1 (ion)
Square pyramidal. The formation of Ph_4P salts can be used in colorimetric determination of V.

Ph_4P salt: [72248-21-6].
$C_{33}H_{28}N_3O_4PSV$ M 641.5
Synth. from NH_4VO_3 and Na_2L at pH 6 in H_2O in the presence of Ph_4PCl. Dark red cryst. solid (EtOH).

Ph_4P salt, monohydrate: [89823-35-8].
Dark red solid.

Ph_4As salt: [72248-20-5].
$C_{33}H_{28}AsN_3O_4SV$ M 685.5
Dark red solid.

Maric, L. *et al, Microchem. J.*, 1979, **24**, 536 (*use, dem V*)
Siroki, M. *et al, J. Inorg. Nucl. Chem.*, 1981, **43**, 1151 (*synth, ir, pmr, uv-vis*)
Galesic, N. *et al, Acta Crystallogr., Sect. C*, 1984, **40**, 378 (*cryst struct, Ph_4P salt*)

$C_9H_5O_3RuS$ IC-006465

Tricarbonyl(phenylthio)ruthenium(*I*)
(Benzenethiolato)tricarbonylruthenium

$[Ru(CO)_3(SPh)]_n$

M 294.2
Believed to be polymeric. Prepd. by treating Dodecacarbonyltriruthenium, IC-008378 in C_6H_6 with S_2Ph_2. Yellow solid. Sol. CCl_4. Mp 158-162° dec. Ir ν_{CO} 2083, 2032, 2027, 2016, 1970 cm^{-1} (CCl_4).

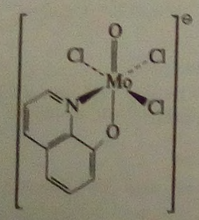
Dimeric form: see *Hexacarbonylbis-μ-(phenylthio) diruthenium*, IC-009734
Johnson, B.F.G. *et al, Nature (London)*, 1967, **213**, 901 (*synth*)
Cetini, G. *et al, J. Organomet. Chem.*, 1968, **15**, P4 (*synth, ir*)

$C_9H_4Cl_3MoNO_2^{\ominus}$ IC-006466

Trichlorooxo(8-quinolinolato-N^1,O^8)molybdate(*V*)(1−), 10Cl

Trichloro-8-hydroxyquinolinatooxomolybdate(V)(1−)

[74707-89-4]



M 362.4 (ion)
Distorted octahedral Mo, with Mo=O 167.3, Mo—N,O 219.8, 203.9, Mo—Cl 235.8, 238.9, 242.8 pm.

8-Hydroxyquinolinium salt: [71936-02-2].
Light-green cryst. (CH_2Cl_2/hexane).

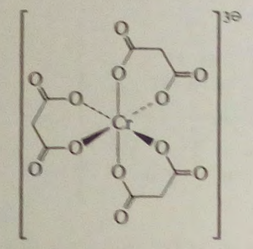
McAuliffe, C.A. *et al, Inorg. Chim. Acta*, 1977, **33**, 5 (*analogues*)
Yamanouchi, K. *et al, Acta Crystallogr., Sect. B*, 1379, **35**, 2326 (*cryst struct, ir, synth*)

$C_9H_6CrO_{12}^{3\ominus}$ IC-006467

Tris(malonato)chromate(*III*)(3−)

Tris[propanedioato(2−)-O,O']chromate(III)(3−), 11Cl, 10Cl, 9Cl

[19203-86-2]



Δ-form

M 358.1 (ion)
Octahedral anion.

Δ-form [58976-25-3]
(−)-form
Δ config. erroneously assigned earlier to (−)-form.
trans(−)[(−)*Tris(1,2-propanediamine)cobalt*(3+)] *salt:*
Not isol. V. sol H_2O. $[\alpha]_D$ −103° (in soln.).

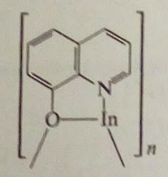
Λ-form
(+)-form
trans(−)[(−)*Tris(1,2-propanediamine)cobalt*(3+)] *salt:* [58927-05-2].
Bronze prisms + $3H_2O$. Struct. consists of columns of alternating Cr and Co complex ions H-bonded together.

(±)-form
Tri-K salt: [70366-25-5].
Dichroic blue-green microcryst. + $3H_2O$.
[23555-18-2]
Butler, K.R. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 251 (*cryst struct, abs config, cd*)
Abdel Khalek, A.A. *et al, J. Inorg. Nucl. Chem.*, 1980, **42**, 1407 (*reactions*)
Basak, A.K. *et al, Bull. Chem. Soc. Jpn.*, 1983, **56**, 318 (*aquation*)

C_9H_6InNO IC-006468

8-(Quinolinolato)indium(*I*)

[57936-49-9]



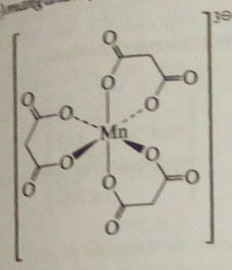
M 258.9
Assoc. in solid and in DMSO soln. Yellow-green hygroscopic solid. V. spar. sol. org. solvs.; sol. DMSO (40°).

Habeeb, J.J. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1815 (*synth, ir*)

$C_9H_6MnO_{12}^{3\ominus}$ IC-006469

Tris[propanedioato(2−)-*O*,*O'*]manganate(*III*)(3−), 10Cl

Tris[malonato]manganate(III)(3−)



M 361.0 (ion)
Pseudo-octahedral. Stable for some time in aq. solns. containing malonic acid or malonates. Solns. slowly reduced to Mn(*II*) and dilution or heating causes hydrol. to Diaquabis[propanedioato(2−)-*O*,*O'*] manganate(*III*)(1−), IC-005018.

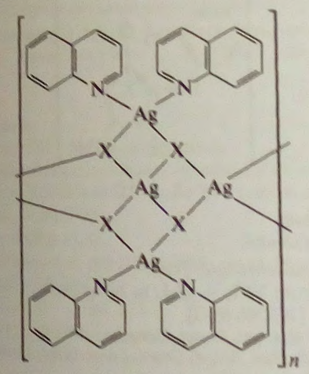
Tri-K salt: [63357-76-6].
Synth. from potassium malonate and $KMn(SO_4)_2.12H_2O$ or $K[Mn(OH_2)_2(malonate)_2].2H_2O$. Air-stable red cryst. + $2H_2O$. High spin d^4 Mn(*III*) complex.

[2261-58-4]
Sivasis, T.N., *Z. Anorg. Allg. Chem.*, 1956, **288**, 288 (*synth*)
Bullock, J.I. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 415 (*synth, ir, uv, magnetism*)
D'Ascenzo, G. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 3109 (*uv*)
Lis, T. *et al, Acta Crystallogr., Sect. B*, 1977, **33**, 1943 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, D2, 130 (*rev, bib*)

C_9H_5AgBrN IC-006470

Bromo(quinoline)silver(*I*), 11Cl

[59413-39-8]



X = Br

M 316.9
Infinite 1-D polymer. Cryst.
Mills, N.K. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 225 (*cryst struct*)

C_9H_5AgClN IC-006471

Chloro(quinoline)silver(*I*), 11Cl

[59413-41-2]

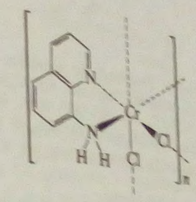
As Bromo(quinoline)silver(*I*), IC-006470 with X = Cl

M 272.4
Infinite 1-D polymer. Cryst.
Mills, N.K. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 225 (*cryst struct*)

$C_9H_6Cl_2CrN_2$ IC-006472

(8-Aminoquinoline)dichlorochromium(*II*), 8Cl

[27435-77-4]



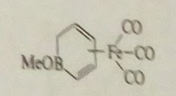
M 267.0
6-Coordinate chloride-bridged polymer. Greenish-yellow, air-sensitive solid. Antiferromagnetic complex: μ_{eff} = 4.28 (300K), $3.59\mu_B$ (90K).

Earnshaw, A. *et al, J. Chem. Soc. A*, 1970, 1840 (*synth, uv, magnetism*)

$C_9H_9BFeO_4$ IC-006473

Tricarbonyl[(3,4,5,6-η)-1,2-dihydro-1-methoxyborin]iron, 10Cl

[72401-05-9]



M 247.8
Precursor for bis(borabenzene)iron. Air-sensitive yellow oil.

Ashe, A.J. *et al, J. Am. Chem. Soc.*, 1979, **101**, 7066 (*synth, nmr, pmr, ms*)

$C_9H_4Cl_6N_3O_3V_2$ IC-006474

μ-Chloroheptachlorotris(2-oxopropanenitrile-*N*) divanadium(*IV*), 11Cl

μ-Chloroheptachlorotris(acetyl cyanide)divanadium(IV)

[104413-80-1]

$Cl_4V[N{\equiv}CC(O)CH_3]{-}Cl{-}VCl_3[N{\equiv}CC(O)CH_3]_2$

M 592.6
Octahedral. Synth. from VCl_4 and 1 mol. acetyl cyanide in pet. ether. Brown solid. Reaction of VCl_4 and excess CH_3COCN gives $VCl_4(CH_3COCN)_2$. Benzoylnitrile analogues are known. Paramagnetic, μ_{eff} = $2.03\mu_B$ (293K).

Nicholls, D. *et al, Inorg. Chim. Acta*, 1986, **115**, L13 (*synth, uv-vis, ir*)

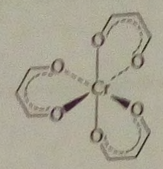
IC-006475

$C_9H_9CrO_6$

Tris(1,3-propanedialato-*O,O'*)chromium, 11CI

Tris(malonaldehydato)chromium(III)

[15636-02-9]



M 265.1

Approx. octahedral. Paramagnetic relaxation agent. Violet-red needles (2-propanol/heptane). Sol. C_6H_6, $CHCl_3$, hot 2-propanol, CH_2Cl_2. Mp 182-183°. Subl., 80-100°. Undergoes electrophilic subst. by NO_2, Br at 2-position.

Collman, J.P. *et al, J. Am. Chem. Soc.*, 1961, **83**, 3529 (*synth, reactions*)
Inorg. Synth., 1968, **8**, 141 (*synth*)
Fatta, A.M. *et al, Inorg. Chem.*, 1971, **10**, 478 (*uv-vis*)
Glick, M.D. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 916 (*cryst struct*)
Eur. Pat., 37 114, (1981); *CA*, 1982, **96**, 40919 (*use*)
Edlund, U. *et al, Org. Magn. Reson.*, 1982, **18**, 207 (*use*)
Berg, E.W. *et al, Inorg. Chem.*, 1983, **22**, 1991 (*synth, ms, ir*)

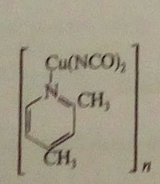
IC-006476

$C_9H_9CuN_3O_2$

Bis(cyanato-*N*)(2,4-dimethylpyridine)copper(*II*), 9CI

Bis(isocyanato)(2,4-lutidine)copper. Dicyanato-2,4-lutidinecopper(II)

[32370-08-4]



M 254.7

Struct. comprises infinite polynuclear chains with approx. square planar Cu. Cyanate groups bridge through the N atom only. Ferromagnetic exchange occurs between Cu(*II*) atoms. Cryst. Insol. H_2O. CAS wrongly assigns this as Bis(cyanato-*O*)(2,4-dimethylpyridine)copper(*II*).

[36605-09-1, 38893-81-1]

Kohout, J. *et al, Monatsh. Chem.*, 1971, **102**, 350 (*synth, magnetism, uv*)
Hrstijova, M. *et al, Chem. Zvesti*, 1974, **28**, 188 (*uv*)
Valach, F. *et al, Collect. Czech. Chem. Commun.*, 1974, **39**, 380 (*cryst struct*)
Kohout, J. *et al, Z. Phys. Chem.*, 1974, **255**, 901 (*magnetism*)

IC-006477

$C_9H_9MnN_3O_3^{\oplus}$

Tris(acetonitrile)tricarbonylmanganese(1+), 9CI

Tricarbonyltris(cyanomethane)manganese(1+)

[55029-83-9]

$[(MeCN)_3Mn(CO)_3]^{\oplus}$

M 262.1 (ion)

Hexafluorophosphate: [54039-60-0].
Synth. from $MnBr(CO)_5$ in refluxing MeCN followed by addition of $[NH_4]PF_6$ in aq. EtOH. Pale-yellow plate-like cryst. (CH_2Cl_2/EtOH). Mp 131-133° dec.

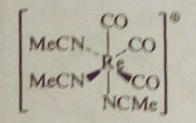
Reimann, R.H. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 808 (*synth, ir, nmr*)
Edwards, D.A. *et al, J. Organomet. Chem.*, 1977, **131**, 73 (*synth, props*)
Kane-Maguire, L.A.P. *et al, Inorg. Chem.*, 1979, **18**, 700 (*synth*)

IC-006478

$C_9H_9N_3O_3Re^{\oplus}$

Tris(acetonitrile)tricarbonylrhenium(1+), 9CI

[66610-17-1]



M 393.3 (ion)

Assigned *fac*-struct. by Reimann *et al.*

Hexafluorophosphate: [66610-18-2].
Synth. from $Re(CO)_5Br$ and $AgPF_6$ in MeCN. Yellow air-stable cryst. Ir ν_{CO} 2045s, 1956s,br cm^{-1} ($CHCl_3$).

Tetrafluoroborate: [64012-16-4].
Synth. from $[nBu_4N]_2[Re_6(CO)_{16}]$ and $AgBF_4$. Cryst. (CH_2Cl_2/heptane, Me_2CO/EtOH).

[75576-70-4]

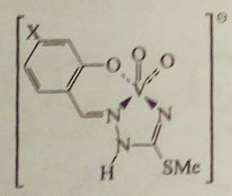
Reimann, R.H. *et al, J. Organomet. Chem.*, 1973, **59**, C24 (*synth, ir, PF_6 salt*)
Chan, L.Y.Y. *et al, Can. J. Chem.*, 1977, **55**, 111 (*synth, cryst struct, ir, BF_4 salt*)
Zdanovitch, V.I. *et al, J. Organomet. Chem.*, 1978, **148**, 63 (*synth, ir, $PF_6^{\ominus}$ salt*)
Kane-Maguire, L.A.P. *et al, Inorg. Chem.*, 1979, **18**, 700 (*synth, ir, PF_6 salt*)

IC-006479

$C_9H_9N_3O_3SV^{\ominus}$

Dioxo(salicylaldehyde-5-methylthiosemicarbazonato)vanadate(*V*)(1−)

[*Methyl* [(2-*hydroxyphenyl*)*methylene*]*hydrazinecarboximidothioato*(2−)-N,N^2,O^2]*dioxovanadate*(V)(*1−*), *11CI*



X = H

M 290.1 (ion)

Square-pyramidal.

NH_4 salt, monohydrate: [76317-57-2].
Synth. from VCl_3 + H_2L in NH_3/EtOH. Cryst.

H-compd.: [105046-69-3].

Ribar, B. *et al, Cryst. Struct. Commun.*, 1980, **9**, 1237 (*cryst struct*)
Petrovic, A.F. *et al, Sov. J. Coord. Chem. (Engl. Transl.)*, 1982, **11**, 239 (*synth, ir, uv-vis*)

IC-006480

$C_9H_9N_3O_3Tc^{\oplus}$

Tris(acetonitrile)tricarbonyltechnetium(*I*)(1+), 12CI

Tricarbonyltris(acetonitrile)technetium(I).
Tricarbonyltris(methyl cyanide)technetium(I)

[113946-05-7]

$[Tc(NCCH_3)_3(CO)_3]^{\oplus}$

M 306.0 (ion)

fac-Octahedral cation. Synth. from $Tc(CO)_5Br$ by reaction with MeCN and $AgPF_6$. Useful synthetic intermediate, e.g. for phosphine complexes.

Hexafluorophosphate: [114375-86-9].
Colourless solid. Sol. CH_2Cl_2; spar. sol. hexane. Mp 138-140°.

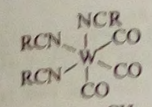
Kaden, L. *et al, Inorg. Chim. Acta*, 1988, **142**, 1 (*synth, ir*)
Findeisen, M. *et al, Inorg. Chim. Acta*, 1988, **142**, 3 (*Tc-99 nmr*)

IC-006481

$C_9H_9N_3O_3W$

Tris(acetonitrile)tricarbonyltungsten

[16800-47-8]



R = CH_3

fac-form

M 391.0

◊ YO7800000.

fac-form [30958-95-3]
Widely used starting material and catalyst. Yellow solid (Me_2CO). Sol. MeCN, $MeNO_2$, sol. with dec. in Me_2CO. Dec. at 135°.

Dobson, G.R. *et al, Inorg. Chem.*, 1962, **1**, 529 (*synth, ir*)
Ross, B.L. *et al, Inorg. Chem.*, 1963, **2**, 1023 (*ir*)
Farona, M.F. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 1895 (*ir*)
Werner, H. *et al, Helv. Chim. Acta*, 1970, **53**, 2002 (*synth, ir*)
Chow, T.J. *et al, J. Am. Chem. Soc.*, 1987, **109**, 797.
Hamilton, E.J.M. *et al, Acta Crystallogr., Sect. C*, 1987, **43**, 1214 (*cryst struct*)

IC-006482

$C_9H_9N_2O_4SV^{\ominus}$

(2,4-Dihydroxybenzaldehyde-5-methylthiosemicarbazonato)dioxovanadate(*V*)(1−)

[*Methyl* [(2,4-*dihydroxyphenyl*)*methylene*]*hydrazinecarboximidothioato*]*dioxovanadate*(V)(*1−*), *11CI*

As Dioxo(salicylaldehyde-5-methylthiosemicarbazonato) vanadate(*V*)(1−), IC-006479 with

X = OH

M 306.1 (ion)

Synth. from Dioxo(salicylaldehyde-5-methylthiosemicarbazonato)vanadate(*V*)(1−), IC-006479 in EtOH and HNO_3 or by reaction of NH_4VO_3 and H_2L in aq. NH_3.

NH_4 salt: [88902-53-8].
Yellow solid. Sol. MeOH, DMF; insol. H_2O, Et_2O.

H deriv.: [105046-68-2].
$C_9H_{10}N_3O_4SV$ M 307.2

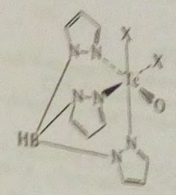
Leovac, V.M. *et al, Transition Met. Chem.*, 1983, **8**, 337 (*synth*)
Petrovic, A.F. *et al, Transition Met. Chem.*, 1986, **11**, 207 (*cryst struct*)

IC-006483

$C_9H_{10}BBr_2N_6OTc$

Dibromo[hydrotris(1*H*-pyrazolato-N^1)borato(1−)-N^2,N^2,N^2]oxotechnetium(*V*), 10CI

[73940-67-7]



X = Br

M 487.7

Octahedral. Synth. from $TcO_4^{\ominus}$ + HBr + ligand, or from $TcOBr_4^{\ominus}$ + ligand. Yellow-brown solid (by chromatog. CH_2Cl_2). Sol. polar org. solvs., insol. H_2O.

Thomas, R.W. *et al, Inorg. Chem.*, 1980, **19**, 2846 (*synth, ir, uv, pmr, ms*)

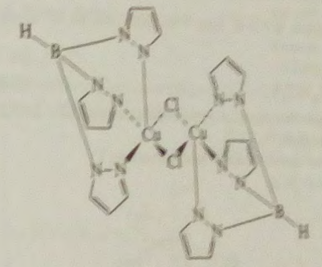
IC-006484

$C_9H_{10}BClCuN_6$

Chloro[hydrotris(1*H*-pyrazolato-N^1)borato(1−)-N^2,N^2,N^2]copper, 10CI

Chloro[hydrotris(1-pyrazolyl)borato]copper(II)

[64811-69-4]



dimer

M 312.0

Dimeric in solid state.

Dimer:
$C_{18}H_{20}B_2Cl_2Cu_2N_{12}$ M 624.0
Emerald green cryst. Sol. $CHCl_3$, CH_2Cl_2; insol. Et_2O.
Square pyramidal at Cu with axial N.

Roundhill, S.G.N. *et al, Inorg. Chem.*, 1979, **18**, 831 (*cryst struct, synth, esr, magnetism, uv-vis*)

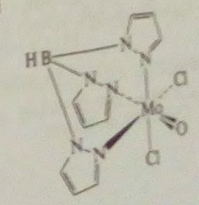
IC-006485

$C_9H_{10}BCl_2MoN_6O$

Dichloro[hydrotris(1*H*-pyrazolato-N^1)borato(1−)-N^2,N^2,N^2]oxomolybdenum(*V*), 11CI

Dichloro[tris(pyrazolyl)borato]oxomolybdenum(V)

[101248-28-6]



M 395.8
Octahedral struct. with disordered O and Cl. Green powder or cryst. (toluene). Paramagnetic.

Lincoln, S. *et al, Inorg. Chem.*, 1986, **25**, 1594 (*synth, uv-vis, cryst struct*)

$C_9H_{10}BCl_2N_6OTc$ IC-006486

Dichloro[hydrotris(1*H*-pyrazolato-N^1)borato(1−)-$N^2,N^{2'},N^{2''}$]oxotechnetium(*V*), 10Cl

Oxodichloro[hydrotris(1-pyrazolyl)borato]technetium(V)

[71835-95-5]

As Dibromo[hydrotris(1*H*-pyrazolato-N^1)borato(1−)-$N^2,N^{2'},N^{2''}$]oxotechnetium(*V*), IC-006483 with

X = Cl

M 398.8
Distorted octahedral geometry. Tc—O 165.6 pm. Synth. from $TcO_4^\ominus$ + $K(HBpyz_3)$ in conc. HCl or by reaction of $TcOCl_4^\ominus$ with $K(HBpyz_3)$. Air stable green cryst. (CH_2Cl_2/toluene). Inert to subst. of Cl ligands in aq. soln. Mp ~220° dec. Intermed. in synth. of rel. compds. e.g. Dichloro[hydrotris(1*H*-pyrazolato-N^1)borato(1−)-$N^2,N^{2'},N^{2''}$]pyridinetechnetium(*III*), IC-008618. Diamagnetic. Oxo ligand induces large structural *trans* effect.

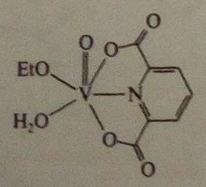
Thomas, R.W. *et al, J. Am. Chem. Soc.*, 1979, **101**, 4581 (*synth, ir, raman, uv, pmr, cryst struct*)
Thomas, R.W. *et al, Inorg. Chem.*, 1980, **19**, 2840 (*synth, ir, uv, pmr, ms*)
Abrams, M.J. *et al, Inorg. Chim. Acta*, 1984, **82**, 125 (*props, reactions*)

$C_9H_{10}NO_7V$ IC-006487

Aquaethoxyoxo[2,6-pyridinedicarboxylato(2−)-N^1,O^2,O^6]vanadium(*V*), 11Cl

Aquaethoxyoxo(dipicolinato)vanadium(V)

[88143-57-1]



M 295.1
Synth. from $H_3O[VO_2dipic]$ and EtOH. Yellow solid.

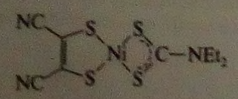
Mimoun, H. *et al, Nouv. J. Chim.*, 1983, **7**, 467 (*synth, ir, pmr*)

$C_9H_{10}N_3NiS_4$ IC-006488

Diethyldithiocarbamato(maleonitriledithiolato)nickel

(Diethylcarbamodithioato-S,S′)[2,3-dimercapto-2-butenedinitrilato(2−)-S,S′]nickel, 9Cl

[63796-65-6]



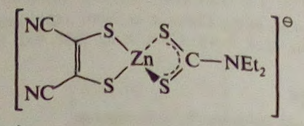
M 347.1
No props. reported.

Dietzsch, W. *et al, Z. Chem.*, 1977, **17**, 191 (*esr*)
Stach, J. *et al, Z. Chem.*, 1978, **18**, 265 (*esr*)

$C_9H_{10}N_3S_4Zn^\ominus$ IC-006489

(*N,N*-Diethyldithiocarbamato)(maleonitriledithiolato)zincate(1−)

(Diethylcarbamodithioato-S,S′)[2,3-dimercapto-2-butenedinitrilato(2−)-S,S′]zincate(1−), 11Cl



M 353.8 (ion)
Tetrahedral Zn.
Ph_4As salt: [102723-66-0].
From $Ph_4As[Zn[S_2C_2(CN)_2]_2]$ and $Zn(S_2CNEt_2)$. Cryst. (Me_2CO/2-propanol). Mp 170-172°.

Leban, I. *et al, Inorg. Chim. Acta*, 1986, **112**, 107 (*synth, cryst struct*)

$C_9H_{11}Cl_2OPPt$ IC-006490

Carbonyldichloro(dimethylphenylphosphine)platinum

As Carbonyldichloro(triethylphosphine)platinum, IC-005776 with

R^1 = Me, R^2 = Ph

M 432.1
cis-form [19618-86-1]
Cryst. ($CHCl_3$/hexane). Mp 184-191°, Mp 181-191° dec.
trans-form [73347-18-9]
Yellow. Obt. in soln. only; readily isom. to *cis*-form.

Jenkins, J.M., *J. Chem. Soc. A*, 1966, 770 (*synth, pmr*)
Smithies, A.L. *et al, J. Organomet. Chem.*, 1968, **12**, 199 (*synth, ir*)
Anderson, G.K. *et al, J. Chem. Res. (S)*, 1979, 120 (*cmr*)
Anderson, G.K. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 1988 (*synth, nmr, ir*)

$C_9H_{12}BMnN_2O_5$ IC-006491

[Bis(dimethylamino)boryl]pentacarbonylmanganese

Pentacarbonylmanganese-bis(dimethylamino)borane

$(OC)_5MnB(NMe_2)_2$

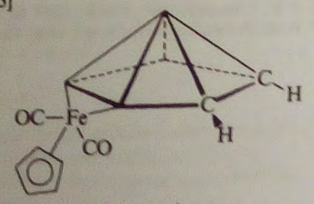
M 293.9
Orange-yellow cryst. Sol. C_6H_6. Mp 60° dec.

Nöth, H. *et al, Angew. Chem., Int. Ed. Engl.*, 1963, **2**, 623 (*synth*)
Nöth, H. *et al, J. Organomet. Chem.*, 1966, **5**, 109 (*synth, ir, B-11 nmr*)

$C_9H_{12}B_4FeO_2$ IC-006492

Dicarbonyl(η⁵-2,4-cyclopentadien-1-yl)[(2,3-η)-heptahydro-4,5-dicarbahexaborato(1−)]iron

[38999-56-3]



1*H not shown*

M 251.2

Intermed. for synthesis of (η⁵-2,4-Cyclopentadien-1-yl)[(2,3,4,5,6-η)-heptahydro-2,5-dicarbahexaborato(1−)-H^{nn}]iron, IC-005749. Bright-yellow.

Sneddon, L.G. *et al, J. Am. Chem. Soc.*, 1972, **94**, 7161; 1973, **95**, 6623 (*synth, ir, ms, pmr, nmr*)

$C_9H_{12}BrMnN_4O$ IC-006493

Bromocarbonyltetrakis(isocyanomethane)manganese, 9Cl

Bromocarbonyltetrakis(methyl isocyanide)manganese

[38833-19-1]

$MnBr(CO)(CNMe)_4$

M 327.0
Synth. from $MnBr(CO)_5$ and MeNC in refluxing THF. Bright-yellow cryst. (CH_2Cl_2/hexane). Mp 176-178°.

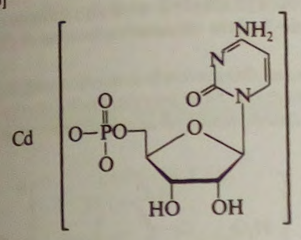
Treichel, P.M. *et al, J. Organomet. Chem.*, 1972, **44**, 339 (*synth, ir, nmr*)
Adams, R.D. *et al, J. Organomet. Chem.*, 1975, **87**, C48 (*synth*)
Treichel, P.M. *et al, J. Organomet. Chem.*, 1976, **122**, 229 (*synth*)

$C_9H_{12}CdN_3O_8P$ IC-006494

[5′-Cytidylato(2−)]cadmium

[Cytidine 5′-(dihydrogen phosphato)]cadmium

[37308-56-8]



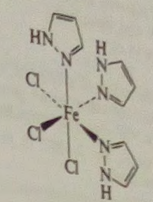
M 433.5
Cryst. + $1H_2O$ (H_2O).
Aqua complex, monohydrate: Aqua[5′-cytidylato(2−)] cadmium monohydrate. 5′-Cytidylic acid, cadmium salt dihydrate
Orthorhombic needles (H_2O). Distorted sq. pyramidal Cd is coord. to N of cytidylato ligand, 3 O of different phosphate groups and O of H_2O.
Aqua complex, sesquihydrate: [67761-40-4]. *5′-Cytidylic acid, cadmium salt hydrate (2:2:5)*
Formed in presence of urea. Monoclinic needles (H_2O). Polymeric: Cd coord. to 4 O of 3 different phosphate groups, to 2 N of cytidylato ligands and to O of H_2O.

Ogawa, M. *et al, Yakugaku Zasshi (J. Pharm. Soc. Jpn.)*, 1972, **92**, 1166 (*synth*)
Goodgame, D.M.L. *et al, Biochem. J.*, 1975, **151**, 467 (*synth, struct, orthorhombic form*)
Clark, G.R. *et al, J. Chem. Soc., Chem. Commun.*, 1975, 697.
Clark, G.R. *et al, Acta Crystallogr., Sect. B*, 1978, **17**, 3484 (*synth, cryst struct, orthorhombic form*)
Shiba, J. *et al, Inorg. Chem.*, 1978, **17**, 3484 (*synth, cryst struct, monoclinic form*)

$C_9H_{12}Cl_3FeN_6$ IC-006495

Trichlorotris(1*H*-pyrazole-N^2)iron(*III*)

[33616-27-2]



M 366.4
fac-Octahedral struct. assigned on basis of spectroscopic data. Orange cryst. Sol. hot EtOH.

Daugherty, N.A. *et al, Inorg. Chem.*, 1968, **7**, 1651 (*synth*)
Cotton, S.A. *et al, J. Chem. Soc. A*, 1971, 1696 (*synth, ir, raman, esr*)

$C_9H_{12}Cl_3NO_2Ti$ IC-006496

(Butanoato-*O*)trichloro(pyridine)titanium(*IV*), 11Cl

[104854-00-4]

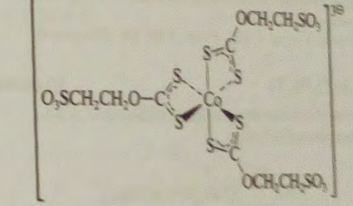
$(Py)TiCl_3(OOCCH_2CH_2CH_3)$

M 320.4
Synth. by reaction of trichlorotitanium butanoate and Py. Yellow solid.

Kapoor, R. *et al, Indian J. Chem., Sect. A*, 1986, **25**, 271 (*synth*)

$C_9H_{12}CoO_{12}S_9^{3\ominus}$ IC-006497

Tris[*O*-(2-sulfoethyl)carbonodithioato(2−)-*S,S*′]cobaltate(*III*)(3−), 10Cl



Δ-form

M 659.7 (ion)
Tri-K salt: [70099-49-9].
Green solid + $2H_2O$ (H_2O). Sol. H_2O.
Δ-form [70116-66-4]
(+)-form
Λ-form [70116-65-3]
(−)-form

Hanson, S.R. *et al, Acta Chem. Scand., Ser. A*, 1979, **33**, 41 (*synth, uv, cd, mcd, resolv*)

$C_9H_{12}N_2O_8V^\ominus$ IC-006498

[L-Aspartato(2−)-N,O^1,O^4][L-glutamato(2−)-N,O^5] vanadate(*III*)(1−), 11Cl

$[(OOCCH_2CHNH_2COO)(OOCCH_2CH_2CHNH_2COO)V]^\ominus$

M 327.1 (ion)

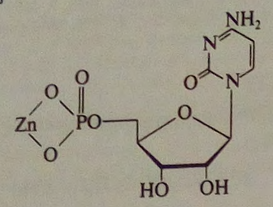
See also Aqua[L-aspartato(2−)-N,O^1,O^4](L-methioninato-N,O)vanadium(*III*), IC-006523. The carboxyl group of glutamate is undissociated. A number of single and mixed salts of aspartic and glutamic acids and methionine are also described.

H compd.: [88314-55-0].
$C_9H_{13}N_2O_8V$ M 328.1
Synth. by Zn reduction of a soln. of V_2O_5 in HCl followed by addn. of aspartic and glutamic acids. Dark green solid. Mp 168° dec. Paramagnetic, $\mu_{eff} = 2.48\mu_B$.

Grecu, I. *et al*, *An. Quim., Ser. B*, 1983, **79**, 18 (*synth, uv-vis, ir, magnetism, thermal anal*)

IC-006499

$C_9H_{12}N_3O_8PZn$
[5′-Cytidylato(2−)]zinc
[37308-60-4]

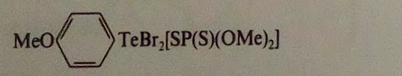


M 386.5
Hydrate: [60866-87-7]. *Aqua[5′-cytidylato(2−)]zinc*
$C_9H_{14}N_3O_9PZn$ M 404.5
Colourless needles. Zn is coord. to N(3) of pyrimidine, to 2 O of phosphate and to O (of water) with additional weak Zn ...O(2) of pyrimidine.

Weitzel, G. *et al*, *Z. Physiol. Chem.*, 1958, **313**, 212 (*stability const*)
Okawa, M. *et al*, *Yakugaku Zasshi (J. Pharm. Soc. Jpn.)*, 1972, **92**, 1166 (*synth, ir*)
Aoki, K., *Biochim. Biophys. Acta*, 1976, **447**, 379 (*cryst struct, hydrate*)
Nishimura, Y. *et al*, *J. Mol. Struct.*, 1986, **146**, 125 (*raman*)

IC-006500

$C_9H_{13}Br_2O_3PS_2Te$
Dibromo[*O,O*-dimethyl phosphorodithioato-*S,S′*](4-methoxyphenyl)tellurium

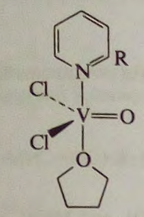


M 551.7
Struct. possesses a bidentate dithiophosphate group with distorted sq. pyr. geometry around Te. Synth. from $ArTeBr_3 + NaS_2P(OMe)_2$. Lemon yellow cryst. ($CHCl_3$/hexane at −4°). Mp 121°.

Chadha, R.K. *et al*, *Organometallics*, 1987, **6**, 813 (*synth, ir, raman, pmr, cryst struct*)

IC-006501

$C_9H_{13}Cl_2NO_2V$
Dichlorooxo(pyridine)(tetrahydrofuran)vanadium(*IV*), 11Cl
[98521-73-4]



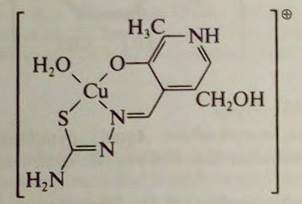
R = H

M 289.0
Trigonal bipyramidal. Synth. from $VOCl_3(THF)_2$ and Py in THF. Green solid. Sol. Me_2O, toluene. Ir ν_{VO} 985 cm^{-1}. Several related compds. also prepd.

Hamid, M.A., *Pak. J. Sci. Ind. Res.*, 1985, **28**, 75; *CA*, **103**, 188378b (*synth, ir, uv-vis*)

IC-006502

$C_9H_{13}CuN_4O_3S^{\oplus}$
Aqua[5-(hydroxymethyl)-2-methylpyridinium-4-carbaldehyde-3-olato thiosemicarbazone-*N,O,S*]copper(*II*) (1+)
Aqua(pyridoxal thiosemicarbazonato)copper(II)(*1+*). *Aqua[2-[[3-hydroxy-5-(hydroxymethyl)-2-methyl-4-pyridiniumyl]methylene]hydrazinecarbothioamidato] copper(1+)*

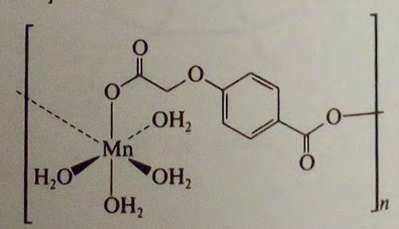


M 320.8 (ion)
Centrosymmetric dimeric cation.
Chloride: [107374-07-2].
Green prismatic cryst. + $1H_2O$. Mp 222° dec. μ_{eff} = $1.81\mu_B$; negligible spin-spin coupling.

Ferrari, M.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 227 (*synth, cryst struct, ir, magnetism*)

IC-006503

$C_9H_{14}MnO_9$
***Catena*-[Tetraaqua(4-carboxylatophenoxyacetato)] manganese(*II*)**
Tetraaqua[4-(carboxymethoxy)benzoato(2−)-O^1] manganese(II), *1ICl*
[89277-23-6]



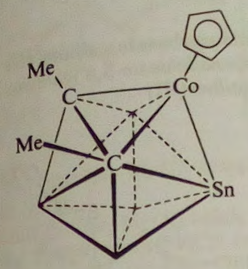
M 321.1

Polymeric struct. Synth. from a hot aq. soln. of 4-carboxyphenoxyacetic acid and $MnSO_4$ in H_2O. Cryst. (H_2O).

Kennard, C.H.L. *et al*, *Inorg. Chim. Acta*, 1984, **82**, 35 (*synth, cryst struct*)

IC-006504

$C_9H_{15}B_4CoSn$
[η^4-2,4-Cyclopentadien-1-yl)[η^4-tetrahydro-*C,C′*-dimethyldicarbastannaheptaborato(2−)]cobalt, 10Cl
[63230-65-9]



M 344.1
closo-. Dark red cryst. Air-stable in solid state, loses tin in soln. Sol. $CHCl_3$, CH_2Cl_2.

Wong, K. *et al*, *Inorg. Chem.*, 1977, **16**, 2053 (*synth, ir, pmr, B-11 nmr, ms*)

IC-006505

$C_9H_{15}BrCoO_3P$
Bromotricarbonyl(triethylphosphine)cobalt
[15977-01-2]

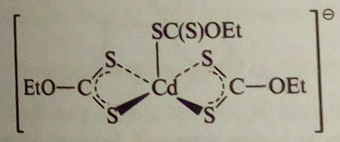
$Et_3PCoBr(CO)_3$

M 341.0
Ir ν_{CO} 1978 cm^{-1} (hexane).

Pankowski, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **264**, 1382 (*synth, ir*)

IC-006506

$C_9H_{15}CdO_3S_6^{\ominus}$
Tris(*O*-ethyldithiocarbonato-*S*)cadmate(1−)
(O-Ethylcarbonodithioato-S)bis(O-ethylcarbonodithioato-S,S′)cadmate(1−), 9Cl. Tris(hydrogen dithiocarbonato) cadmate(1−) O,O,O-triethyl ester, 8Cl



M 476.0 (ion)
Square pyramidal anion.
Et_4N salt: [39043-89-5].
Pale yellow prisms.

[31284-60-3]

Shul'man, V.M. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1967, 154 (*stability const*)
Hunt, M.R. *et al*, *Aust. J. Chem.*, 1971, **24**, 53 (*ir*)
Hoskins, B.F. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 875 (*synth, cryst struct*)
Haberkorn, R.A. *et al*, *Inorg. Chem.*, 1976, **15**, 2408 (*Cd-113 nmr*)

IC-006507

$C_9H_{15}ClCoO_3P$
Tricarbonylchloro(triethylphosphine)cobalt
[15977-02-3]

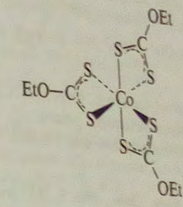
$Et_3PCoCl(CO)_3$

M 296.5
Ir ν_{CO} 1976 cm^{-1}(hexane).

Pankowski, M. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **264**, 1382 (*synth, ir*)

IC-006508

$C_9H_{15}CoO_3S_6$
Tris(*O*-ethyldithiocarbonato)cobalt(*III*)
Tris(O-*ethylcarbonodithioato*-S,S′)*cobalt*(III). *Tris*(hydrogen dithiocarbonato)*cobalt*-O,O,O-*triethyl ester*, *8Cl*. *Tris*(*ethylxanthato*-S,S′)*cobalt*(III)
[15277-79-9]

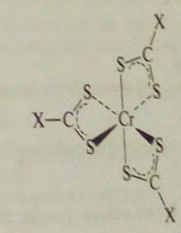


M 422.5
Octahedral. Dark green cryst. solid. Dec. at 130-150°.

Inorg. Synth., 1967, **10**, 42 (*synth*)

IC-006509

$C_9H_{15}CrO_3S_6$
Tris(*O*-ethyldithiocarbonato)chromium(*III*)
Tris(O-*ethyl carbonodithioato*-S,S′)*chromium*(III), *9Cl*. *Tris*(*ethylxanthato*)*chromium*(III). *Chromium*(III) *xanthate*
[15276-08-1]



X = OEt

M 415.6
Distorted octahedron about Cr. Dark blue cryst. (Py aq.). Insol. H_2O; sol. org. solvs.

Merlino, S. *et al*, *Acta Crystallogr., Sect. B*, 1972, **28**, 972 (*cryst struct*)

IC-006510

$C_9H_{15}CrS_9$
Tris(ethyltrithiocarbonato)chromium(*III*)
Tris(*monoethyl carbonotrithioato*-S,S′)*chromium*(III), *10Cl*. *9Cl*. *Tris*(*ethyl carbonotrithioato*-S,S′)*chromium*. *Tris*(*ethylthioxanthato*)*chromium*(III)
[31316-05-9]
As Tris(*O*-ethyldithiocarbonato)chromium(*III*), IC-006509 with

X = SEt

M 463.8

Octahedral at Cr. Green(?) cryst.
Villa, A.C. *et al. Acta Crystallogr., Sect. B*, 1974, **30**, 2788 (*cryst struct*)
Vella, P. *et al. J. Inorg. Nucl. Chem.*, 1978, **40**, 613 (*electrochem*)

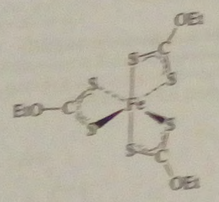
IC-006511

$C_9H_{15}FeO_3S_6$

Tris(*O*-ethyl dithiocarbonato)iron(*III*)

Tris(*O*-ethyl carbonodithioato-*S,S'*)iron(III). *Tris*(ethyl xanthato)iron(III)

[19543-92-1]



M 419.4
Octahedral. Electrolytic synth. from $(EtOCS_2)_2$ + Fe electrolytic. Black hexagonal prisms. μ_{eff} = 2.72μ_B (296K); predominantly low spin Fe(*III*).

[21157-64-6]
Ewald, A.H. *et al. Inorg. Chim.*, 1969, **8**, 1837 (*magnetism*)
Hoskins, B.F. *et al. J. Chem. Soc., Chem. Commun.*, 1970, 45 (*cryst struct*)
Coucouvanis, D., *Prog. Inorg. Chem.*, 1970, **11**, 233; 1979, **26**, 301 (*rev., bibl*)
Cotton, S.A. *et al. J. Chem. Soc. A*, 1971, 869 (*esr*)
Tapia, C.A. *et al. Inorg. Chim. Acta*, 1977, **23**, 165 (*magnetism*)
Lopez, A.D. *et al. An. Quim.*, 1978, **74**, 1466 (*ir, uv-vis*)
Nitta, G.H. *et al. Thermochim. Acta*, 1982, **52**, 31 (*dec*)
Wajda, S. *et al. Radiochem. Radioanal. Lett.*, 1983, **55**, 195 (*synth, mössbauer, magnetism*)
Casey, A.T. *et al. J. Coord. Chem.*, 1988, **16**, 375 (*synth*)

IC-006512

$C_3H_6FeO_3$

Iron(*III*) lactate

Iron(III) *2-hydroxypropanoate. Ferric lactate*

[20563-41-1]

$Fe(OOCCH(OH)CH_3)_3$

M 323.0
Lipase inhibitor. Brown amorph. powder; deliquescent. Sol. H_2O.
Gmelin Handbook Inorg. Chem., Syst. No. 59, 1930, **B3**, 532 (*rev, bibl*)

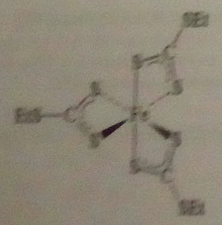
IC-006513

$C_9H_{15}FeS_6$

Tris(ethyl trithiocarbonato)iron

Tris(monoethylcarbonotrithioato-*S',S''*)iron(III), *9CI*. *Tris*(ethylthioxanthato)iron(III)

[21157-64-6]



M 467.6

Black cryst. (CH_2Cl_2). Sol. CH_2Cl_2, $CHCl_3$, CS_2. Mp 90°. μ_{eff} = 2.58μ_B (296K); 2.19μ_B (109K). High-spin low-spin equilibrium. Dec. in soln. at r.t. to afford diamagnetic dimer Bis[μ-(ethanethiolato)]bis[μ-(ethylcarbonotrithioato-*S',S''*)] bis(ethylcarbonotrithioato-*S',S''*)diiron(*III*), IC-009437.
Ewald, A.H. *et al. Aust. J. Chem.*, 1968, **21**, 927 (*synth, magnetism, uv-vis*)
Coucouvanis, D. *et al. J. Am. Chem. Soc.*, 1969, **91**, 761 (*reaction*)
Geetharani, K. *et al. Spectrochim. Acta, Part A*, 1974, **30**, 2165 (*ir*)

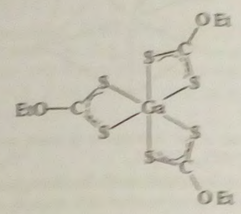
IC-006514

$C_9H_{15}GaO_3S_6$

Tris(*O*-ethyldithiocarbonato)gallium(*III*)

Tris(O-ethylcarbonodithioato-*S,S'*)gallium, *11CI*. *Tris*(O-ethylxanthato)gallium(III)

[94553-05-6]



M 433.3
Geometry at Ga intermed. between octahedral and tbp. Synth. from $GaCl_3$ and KS_2COEt. Colourless cryst. (C_6H_6/hexane). Dec. slowly by acid.
Delphine, H., *Ann. Chim.*, 1951, **6**, 645 (*synth*)
Hoskins, B.F. *et al. Inorg. Chim. Acta*, 1984, **90**, 197 (*synth, cryst struct, ir, pmr, cmr*)

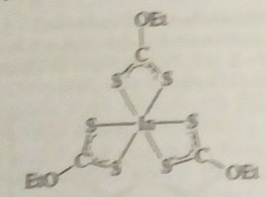
IC-006515

$C_9H_{15}InO_3S_6$

Tris(*O*-ethyldithiocarbonato)indium(*III*)

Tris(O-ethylxanthato)indium(III)

[21630-86-4]

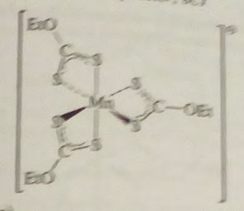


M 478.4
C_3 geometry at indium intermed. between octahedral and trigonal prismatic. Colourless cryst. (EtOH/$CHCl_3$ 2:1). Dec. slowly in air. Insol. H_2O; spar. sol. Et_2O, EtOH, hexane; sol. $CHCl_3$, THF, CS_2. Mp 130-150° dec.
Sutton, G.L., *J. R. Austral. Chem. Inst.*, 1950, **17**, 249 (*synth*)
Delphine, H., *Anal. Chem.*, 1951, **6**, 645 (*synth*)
Inorg. Synth., 1967, **10**, 42 (*synth*)
Hansen, S.R. *et al. Acta Chem. Scand., Ser. A*, 1979, **33**, 41 (*ir*)
Hoskins, B.F. *et al, Inorg. Chim. Acta*, 1984, **90**, 197 (*cryst struct, ir, pmr, cmr*)

$C_9H_{15}MnO_3S_4^{\ominus}$

Tris(*O*-ethyldithiocarbonato)manganate(*II*) IC-006516

Tris(O-ethylcarbonodithioato-*S,S'*)manganate(II)(*1–*). *11CI*. *Tris*(ethylxanthato)manganate(II). *Tris*(dithiocarbonato) *manganate(1–)O,O,O-triethyl ester, 8CI*



M 418.5 (ion)
Octahedral at Mn; high spin Mn(*II*) complex.
Et_4N salt: [33751-74-5].
Synth. from KSC(S)OEt, Mn(*II*) halide and $[Et_4N]Cl$ in H_2O under N_2. Yellow cryst. (MeCN or CH_2Cl_2/Et_2O). μ_{eff} = 6.0μ_B at r.t.
Holah, G.D. *et al, Can. J. Chem.*, 1971, **49**, 2726 (*synth, ir, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 133 (*rev, bibl*)

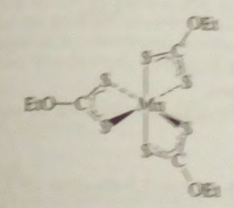
IC-006517

$C_9H_{15}MnO_3S_4$

Tris(*O*-ethyldithiocarbonato)manganese(*III*)

Tris(O-ethylcarbonodithioato-*S,S'*)manganese(III), *9CI*. *Tris*(ethylxanthato)manganese(III)

[105936-08-1]



M 418.5
Octahedral complex. Synth. by electrochemical oxidn. of $Mn(S_2COEt)_2$ in Me_2CO. Purple-brown solid. μ_{eff} = 4.82μ_B.
Casey, A.T., *Transition Met. Chem.*, 1986, **11**, 366 (*synth, ir, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 133 (*rev, bibl*)

IC-006518

$C_9H_{15}O_3PbS_4^{\ominus}$

Tris(*O*-ethyl dithiocarbonato)plumbate(1–)

Tris(O-ethyl carbonodithioato-*S,S'*)plumbate(*1–*). *11CI*. *Tris*(ethylxanthato)plumbate(II)

$[Pb(S_2COEt)_3]^{\ominus}$

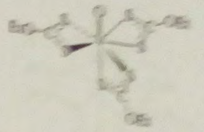
M 570.8 (ion)
Et_4N salt: [31284-53-4].
Formed from an equimolar mixt. of K ethylxanthate, Pb ethylxanthate and $[Et_4N]Br$. Cryst.
Hon, M.R. *et al, Aust. J. Chem.*, 1971, **24**, 53 (*synth, ir*)
Hoskins, B.F. *et al. Aust. J. Chem.*, 1982, **35**, 2423 (*cryst struct*)

$C_9H_{15}O_3S_3V$

Tris(*O*-ethyldithiocarbonato)oxovanadium(*V*) IC-006519

Tris(O-ethyl carbonodithioato-*S,S'*)oxovanadium(V). *11CI*. *Tris*(ethylxanthato)oxovanadium(V). *Oxotris(ethylxanthato) vanadium(V)*

[84140-91-1]



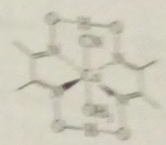
M 410.5
Distorted pentagonal bipyramid with apical O. Synth. from $NaVO_3$ and KS_2COEt in CH_2Cl_2/aq. at 10° C. Yellow-orange/red-brown dichroic solid. Sol. CH_2Cl_2. Mp 88-91° Corresp. methylxanthate is also known.
Garlow, G. *et al, Z. Anorg. Allg. Chem.*, 1982, **492**, 69–102, **498**, 85 (*synth, ir, uv-vis, cryst struct, pmr*)

$C_9H_{18}CaN_3O_3$

Aquo(pentadeuteriodimethylglycinato)(glycinato)calcium(II)

Aquo(pentadeuteriodimethylglycinato)(glycinato)calcium(II). Aquo[(2,2-dimethyl-d6)propionato-N,O][glycinato]calcium(II), *8CI*

[15827-38-8]



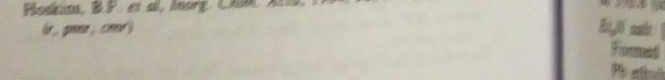
M 359.5
Model for vitamin B_{12} systems. Yellow solid.
Yamauchi, O. *et al. Bull. Chem. Soc. Jpn.*, 1977, **50**, 82 (*synth, ir*)
Abrahams, S. *et al. Inorg. Chim. Acta*, 1982, **64**, L249 (*synth, cryst struct*)

$C_9H_{18}CaN_3O_3S_3$

catena-[L-Methionyl-L-methylcysteinato-*N,N',O,O',S'*] hydridocopper(II)

[N-L-Methionyl-S-methyl-L-cysteinato(2–)-*κN,N',O,O',S'*] copper(II)

[102784-02-1]



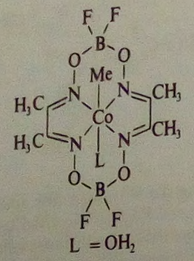
M 327.9
Cu atom is square pyramidal with no Cu···S interaction; chain struct. in which each dipeptide molecule coordinates with 3 different Cu(II) and each Cu(II) is bonded to 3 different peptide molecules. Cryst.
Perin, L.D. *et al. J. Chem. Soc., Dalton Trans.*, 1986, 499 (*cryst struct, electrochem*)

$C_9H_{17}B_2CoF_4N_4O_5$ IC-006522

Aqua[bis[μ-[(2,3-butanedione dioximato)(2−)-*O*:*O*′]]]tetrafluorodiborato(2−)-*N*,*N*′,*N*″,*N*‴]methylcobalt, 10CI

[Tetrafluorobis[dimethylglyoximato(2−)]diborato]aquomethylcobalt

[53729-64-9]



M 417.8

Vitamin B_{12} analogue. Yellow cryst. (MeOH aq.). Sol. H_2O. Co–Me bond cleaved by light, OH^- and Hg^{2+}. H_2O ligand easily replaced by Lewis bases, e.g. Py.

Schrauzer, G.N. *et al*, *J. Am. Chem. Soc.*, 1966, **88**, 3738 (*synth*)
Adin, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 653.
Cartano, A.V. *et al*, *Bioinorg. Chem.*, 1977, **7**, 351 (*synth*)
Brown, K.L., *J. Am. Chem. Soc.*, 1979, **101**, 6600 (*pmr, props*)

$C_9H_{17}N_2O_7SV$ IC-006523

Aqua[L-aspartato(2−)-*N*,*O*^{1},*O*^{4}](L-methioninato-*N*,*O*)vanadium(*III*), 11CI

[88325-14-8]

$(H_2O)[OOCCH_2CH(NH_2)COO][MeSCH_2CH_2CH(NH_2)COO]V$

M 348.2

Synth. by Zn reduction of VCl_4 in HCl followed by addn. of aspartic acid and methionine. Dark green solid. Mp 156-158° dec. Paramagnetic; $\mu_{eff} = 2.81\mu_B$. Several rel. compds. also descr.

Grecu, I. *et al*, *An. Quim., Ser. B*, 1983, **79**, 18 (*synth, uv-vis, ir, magnetism, thermal anal*)

$C_9H_{18}AlCl_2N$ IC-006524

(Di-*tert*-butylmethyleneamino)aluminium dichloride

(1-tert-Butyl-2,2-dimethylpropylideniminato)dichloroaluminium

dimer

R = $C(CH_3)_3$

M 238.1

Dimeric.

Dimer: [30153-69-6]. *Bis[μ-(1-tert-butyl-2,2-dimethylpropylideniminato)]tetrachlorodialuminium* $C_{18}H_{36}Al_2Cl_4N_2$ M 476.2

Synth. from $AlCl_3$ and $^tBu_2C{=}NLi$. White moisture-sensitive cryst. (toluene/heptane). Mp 124-126°.

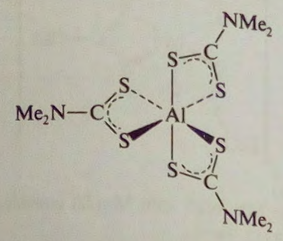
Snaith, R. *et al*, *J. Chem. Soc. A*, 1970, 2635 (*synth, ir, ms*)

$C_9H_{18}AlN_3S_6$ IC-006525

Tris(*N*,*N*-dimethyldithiocarbamato)aluminium

Tris(dimethylcarbamodithioato-S,S′)aluminium

[60955-53-5]



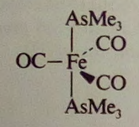
M 387.6

Monomeric in C_6H_6. Synth. from $Al(NMe_2)_3 + CS_2$. Used in photographic industry. Colourless cryst. + $1CH_2Cl_2$ (CH_2Cl_2/pentane). Mp 170° dec.

Nöth, H. *et al*, *Chem. Ber.*, 1983, **116**, 3552 (*synth, ir, Al-27 nmr, cryst struct*)

$C_9H_{18}As_2FeO_3$ IC-006526

Tricarbonylbis(trimethylarsine)iron, 8CI



M 379.9

trans-form [30230-17-2]
Cryst. (hexane).

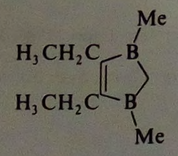
Bigorgne, M., *J. Organomet. Chem.*, 1970, **24**, 211 (*synth, ir*)

$C_9H_{18}B_2$ IC-006527

4,5-Diethyl-2,3-dihydro-1,3-dimethyl-1*H*-1,3-diborole, 11CI

4,5-Diethyl-1,3-dimethyl-Δ^4-1,3-diborolene

[81620-71-5]



M 147.8

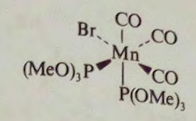
Used in synth. of oligodecker sandwich complexes, such as μ-(4,5-Diethyl-1,3-dimethyl-1,3-diborolenyl)bis[(η^5-cyclopentadienyl)nickel], IC-010282. Colourless air-sensitive liq. Sol. C_6H_6. Bp_{30} 73-75°.

Siebert, W. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 148; 1985, **24**, 943.
Edwin, J. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 2582 (*synth, nmr*)
Edwin, J. *et al*, *Organometallics*, 1983, **2**, 1666 (*cmr*)
Siebert, W. *et al*, *Z. Naturforsch., B*, 1985, **40**, 326.

$C_9H_{18}BrMnO_9P_2$ IC-006528

Bromotricarbonylbis(trimethylphosphite-*P*)manganese, 9CI

[52841-89-1]



M 467.0

Synth. from $Mn(COCH_3)(CO)_3[P(OMe)_3]_2$ and Br_2 at −8° in CCl_4. Orange cryst. Mp 110°. Ir ν_{CO} 2052, 1975, 1939 cm^{-1}.

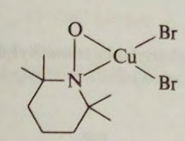
Treichel, P.M. *et al*, *J. Organomet. Chem.*, 1969, **17**, P37 (*synth, ir, pmr*)
Reimann, R.H., *J. Chem. Soc., Dalton Trans.*, 1973, 841 (*synth, ir, pmr*)

$C_9H_{18}Br_2CuNO$ IC-006529

Dibromo(1-hydroxy-2,2,6,6-tetramethylpiperidinato-*N*^{1},*O*^{1})copper(*II*)

Copper(II) bromide 2,2,6,6-tetramethylpiperidinyl-1-oxy

[113132-33-5]



M 379.6

Strong antiferromagnetically coupled copper(*II*) nitroxyl species. First metal nitroxyl complex in which both the oxygen and the nitrogen co-ordinate to the metal centre. First example of a 3-membered metallacycle including copper. Dark brown cryst. (CH_2Cl_2/Et_2O). μ_{eff} = $0.15\mu_B$.

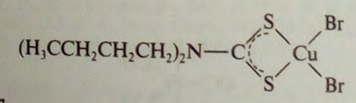
Caneschi, A. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 2307 (*cryst struct, synth, magnetism*)

$C_9H_{18}Br_2CuNS_2$ IC-006530

Dibromo(*N*,*N*-dibutyldithiocarbamato)copper(*III*)

Dibromo(dibutylcarbamodithioato-S,S′)copper(III), 9CI

[20249-26-7]



M 427.7

Dark violet, needle shaped cryst. Sol. $CHCl_3$, CH_2Cl_2; insol. Et_2O. Mp 99°.

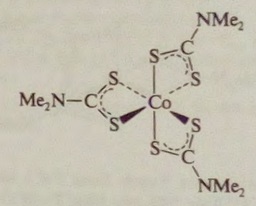
Beurskens, P.T. *et al*, *Inorg. Chem.*, 1968, **7**, 810 (*cryst struct, ir, esr, synth, uv, magnetism*)

$C_9H_{18}CoN_3S_6$ IC-006531

Tris(*N*,*N*-dimethyldithiocarbamato)cobalt(*III*)

Tris(dimethylcarbamodithioato-S,S′)cobalt(III), 10CI

[23677-76-1]



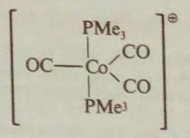
M 419.5

Green solid. Sol. $CHCl_3$.

Gahan, L.R. *et al*, *Inorg. Chem.*, 1979, **18**, 933 (*synth, uv*)

$C_9H_{18}CoO_3P_2^{\oplus}$ IC-006532

Tricarbonylbis(trimethylphosphine)cobalt(1+)



M 295.1 (ion)

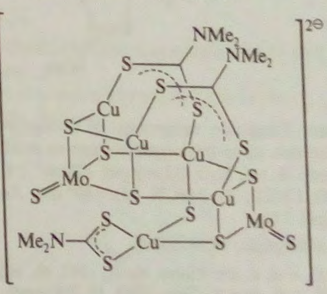
Tetraphenylborate: [52691-19-7].
$C_{33}H_{38}BCoO_3P_2$ M 614.3
White solid. Sol. CH_2Cl_2, Me_2CO. Mp 207° dec. Ir ν_{CO} 1998 cm^{-1} (Me_2CO).

[38670-37-0]

Attali, S. *et al*, *Inorg. Chim. Acta*, 1972, **6**, 475 (*synth, ir, pmr*)
Arabi, M.S. *et al*, *J. Organomet. Chem.*, 1974, **67**, 109 (*synth, ir*)

$C_9H_{18}Cu_5Mo_2N_3S_{14}^{2\ominus}$ IC-006533

[Bis[μ-(dimethylcarbamodithioato-*S*:*S*′)](dimethylcarbamodithioato-*S*,*S*′)pentacuprate]hexa-μ$_3$-thioxodithioxodimolybdate(2−), 12CI



M 1126.7 (ion)

Bis-Et$_4$N salt: [123565-75-3].
Violet-black cryst. + $2H_2O$ (DMF/Et_2O). Sol. DMF; insol. Et_2O.

Lei, X. *et al*, *Inorg. Chem.*, 1989, **28**, 4302 (*synth, cryst struct, ir*)

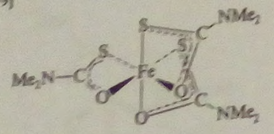
IC-006534

$C_9H_{18}FeN_3O_2S_3$

Tris(*N,N*-dimethylthiocarbamato)iron(*III*)

Tris(dimethylcarbamothioato-O,S)iron, 10CI

[60648-07-9]



M 368.3

fac-Octahedral isomer. Synth. from $FeCl_3.6H_2O$ in MeOH + $[Me_2NCOS][Me_2NH_2]$ or from $Fe_2(CO)_9$, $[Me_2NCOS]_2$ + S_8. Heat sensitive dark red solid. May be stored at 0° under N_2 as solid or soln. at r.t. Spin equilm. system (6 to 300K); a crystalline modification remains high spin down to 10K.

[61375-77-7]

Nakajima, H. *et al. Inorg. Nucl. Chem. Lett.*, 1976, **12**, 689 (*synth, magnetism*)
Kuzuz, K.R. *et al. Inorg. Chem.*, 1977, **16**, 594 (*synth, magnetism, mösbauer*)
Ahmed, J. *et al. Inorg. Chem.*, 1977, **16**, 935 (*struct*)
Springsteen, K.R.M. *et al. Inorg. Chim. Acta*, 1977, **23**, 13 (*synth*)
Perry, D.L. *et al. J. Inorg. Nucl. Chem.*, 1980, **42**, 1356 (*ir, electrochem*)
Perry, D.L. *et al. J. Chem. Soc., Dalton Trans.*, 1981, 1294 (*magnetism, esr*)

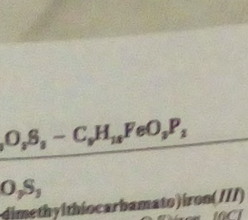
IC-006535

$C_9H_{18}FeN_3S_6$

Tris(*N,N*-dimethyldithiocarbamato)iron(*III*), 8CI

Tris(dimethylcarbamodithioato-S,S')iron(III), 11CI. Ferbam, BSI. Fermate

[14484-64-1]



M 416.5

Octahedral. Fungicide, component of Trimanzone. Black powder; dec. upon prolonged storage or in contact with moisture. Sl. sol. H_2O (13 mg per 100cm³, r.t.). Sol. Me_2CO, $CHCl_3$, Py, MeCN. Mp 180° dec. Acidic in aq. soln. (pH 5.0).

▷ Irritant. Mutagenic. NO8750000.

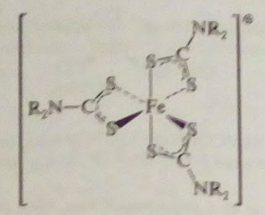
Hodge, H.C. *et al. J. Am. Pharm. Assoc.*, 1952, **41**, 662 (*tox*)
White, A.H. *et al. Aust. J. Chem.*, 1963, **17**, 294 (*synth, magnetism*)
Ewald, A.H. *et al. Inorg. Chem.*, 1969, **8**, 1837 (*magnetism*)
Couccouvanis, D., *Prog. Inorg. Chem.*, 1970, **11**, 233; 1979, **26**, 301 (*rev, bibl*)
Pasek, E.A. *et al. Inorg. Chem.*, 1972, **11**, 259 (*oxidation*)
Chant, R. *et al. Inorg. Chem.*, 1975, **14**, 1894 (*electrochem*)
Hall, G.R. *et al. Inorg. Chem.*, 1976, **15**, 607 (*ir, magnetism*)
Nicholas, M.L. *et al. J. Assoc. Off. Anal. Chem.*, 1976, **59**, 1266 (*raman*)
Beinroht, E. *et al. Collect. Czech. Chem. Commun.*, 1980, **45**, 1785 (*pmr*)

$C_9H_{18}FeN_7S_6$ ® IC-006536

Tris(*N,N*-dimethyldithiocarbamato)iron(*IV*)(1+)

Tris(dimethylcarbamodithioato-S,S')iron(IV)(1+), 9CI

[46935-65-3]



R = Me

M 416.5 (ion)

Octahedral low spin Fe(*IV*) complex. Synth. by BF_3/O_2 oxidation of $Fe(S_2CNMe_2)_3$. Analogues are known.

Tetrafluoroborate: [35270-32-7].
Black.

Pasek, E.A. *et al. Inorg. Chem.*, 1972, **11**, 259 (*synth, mösbauer*)
Pasek, E.A. *et al. Inorg. Chim. Acta*, 1977, **21**, 23.

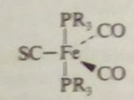
IC-006537

$C_9H_{18}FeO_2P_2S$

Dicarbonyl(thiocarbonyl)bis(trimethylphosphine)iron

(Carbonothioyl)dicarbonylbis(trimethylphosphine)iron, 11CI

[102566-46-1]



R = Me

M 308.1

Air-stable yellow cryst. (pentane). Mp 180-182°. Ir ν_{CO} 1930, 1870 cm^{-1}; ν_{CS} 1215 cm^{-1}(nujol).

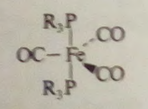
Touchard, D. *et al. J. Chem. Soc., Chem. Commun.*, 1986, 37 (*synth, ir, ms, pmr, cmr, P-31 nmr*)
Organomet. Synth., 1988, **4**, 149 (*synth, ir, pmr, cmr, P-31 nmr, ms*)

IC-006538

$C_9H_{18}FeO_3P_2$

Tricarbonylbis(trimethylphosphine)iron, 9CI, 8CI

[25921-55-5]



R = Me

M 292.0

Trigonal bipyramidal with axial P.

trans-form [30230-16-1]

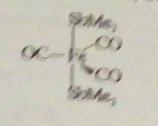
Air-sensitive colourless cryst. (hexane). Solns. v. air-sensitive. Mp 40°. Sublimes near r.t. Ir ν_{CO} 1863 cm^{-1}.

Strohmeier, W. *et al. Chem. Ber.*, 1969, **102**, 3613 (*synth*)
Bigorgne, M., *J. Organomet. Chem.*, 1970, **24**, 211 (*ir, raman*)
Pankowski, M. *et al. J. Organomet. Chem.*, 1976, **110**, 331 (*synth*)
Karsch, H.H. *et al. Chem. Ber.*, 1977, **110**, 2200 (*synth, nmr*)
Grobe, J. *et al. Z. Naturforsch., B*, 1981, **36**, 8 (*synth*)
Inorg. Synth., 1989, **25**, 155; 1990, **28**, 177 (*synth*)

IC-006539

$C_9H_{18}FeO_3Sb_2$

Tricarbonylbis(trimethylstibine)iron, 8CI



M 473.5

trans-form [30230-18-3]

Cryst. (hexane).

Bigorgne, M., *J. Organomet. Chem.*, 1970, **24**, 211 (*synth, ir, raman*)

IC-006540

$C_9H_{18}FeO_6P_2S$

Dicarbonyl(thiocarbonyl)bis(trimethyl phosphite)iron

(Carbonothioyl)dicarbonylbis(trimethyl phosphite-P)iron

[110904-47-7]

As Dicarbonyl(thiocarbonyl)bis(trimethylphosphine)iron, IC-006537 with

R = OMe

M 404.0

Yellow cryst. Ir ν_{CO} 1970vs, 1910vs; ν_{CS} 1240vs cm^{-1} (nujol).

Touchard, D. *et al, Organometallics*, 1988, **7**, 67 (*synth, ir, pmr, ms*)

IC-006541

$C_9H_{18}FeO_9P_2$

Tricarbonylbis(trimethyl phosphite-*P*)iron, 9CI

Tricarbonylbis(phosphorous acid)iron hexamethyl ester, 8CI

[14949-85-0]

M 388.0

trans-form [19457-84-2]

Light-yellow cryst. (pentane). Mp 73-74°.

Pollick, P.J. *et al, J. Organomet. Chem.*, 1968, **14**, 469 (*synth*)
Mosbo, J.A. *et al, J. Magn. Reson.*, 1972, **8**, 243 (*pmr*)
Ginderow, D., *Acta Crystallogr., Sect. B*, 1974, **30**, 2798 (*struct*)
Darensbourg, D.J. *et al, Inorg. Chem.*, 1974, **13**, 2135 (*ir*)
Graf, J.L. *et al, Organometallics*, 1982, **1**, 837 (*ir*)

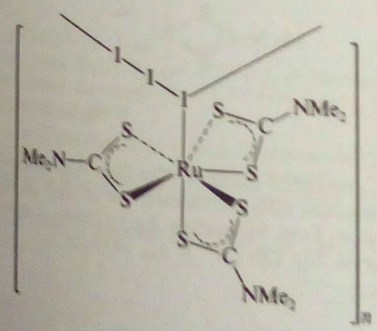
IC-006542

$C_9H_{18}I_3N_3RuS_6$

Tris(*N,N*-dimethyldithiocarbamato)(triiodo)ruthenium(*IV*)

Tris(dimethylcarbamodithioato-S,S')(triiodo)ruthenium(IV), 10CI

[60949-75-9]



M 842.4

Distorted pentagonal bipyramid at Ru. Struct. contains infinite planar chains of iodine atoms; the short I—I distance is only 13 pm longer than in solid molecular I_2. Prepd. by the oxidation of Tris(*N,N*-dimethyldithiocarbamato)ruthenium(*III*), IC-006546 with I_2 in CH_2Cl_2. R_{Ru-I} 275.2; $R_{Ru-S_{ax}}$ 239.7; I—I 283.4; I..I 397.9 pm. Yellow cryst., diamagnetic.

Matson, R.M. *et al, Inorg. Chem.*, 1977, **16**, 488 (*synth, pmr, cryst struct*)

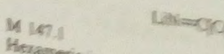
IC-006543

$C_5H_{10}LiN$

***N*-Lithio(6-*tert*-butyl)azinane**

Lithium di-tert-butylmethyleneamide. Di-tert-butylmethyleneamidolithium

[95218-73-8]



M 147.1

Hexameric in cryst. state.

Hexamer [72859-98-7]. *Hexakis(μ$_3$-(2,2,4,4-tetramethyl-3-pentanimino))hexalithium*

$C_{30}H_{60}Li_6N_6$ M 883.1

White microcryst. powder or pale-yellow cryst. (pentane/hexane). Sol. hydrocarbons, ethers. Ir $\nu_{C=N}$ 1593 cm^{-1}.

Hexamethylphosphoramide complex: [95218-71-6].

$C_{15}H_{36}LiN_4OP$ M 326.3

Yellow cryst. (pentane/hexane). Mp 128-130°.

Monomeric in soln. Dimeric in cryst. state.

[95218-70-5]

Clegg, W. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1309 (*synth, struct, ir*)
Barr, D. *et al, Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 328 (*synth, struct, pmr, Li-7 nmr*)
Reed, D. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 557 (*props, Li-7 nmr*)
Barr, D. *et al, Magn. Reson. Chem.*, 1986, **24**, 713 (*pmr, Li-7 nmr*)
Barr, D. *et al, J. Chem. Soc., Dalton Trans.*, 1987, 2141 (*deriv, cryst struct*)

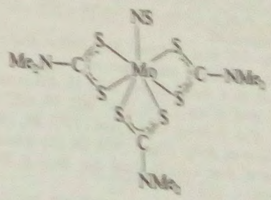
IC-006544

$C_9H_{18}MoN_4S_5$

Tris(*N,N*-dimethyldithiocarbamato)(thionitrosyl)molybdenum

Tris(dimethylcarbamodithioato-S,S')(thionitrosyl)molybdenum, 10CI

[54171-62-9]



M 502.6

Synth. from $MoN(S_2CNMe_2)_3$ + S. Orange-yellow, air-stable cryst. (CH_2Cl_2/MeOH). Sol. $CHCl_3$, CH_2Cl_2.

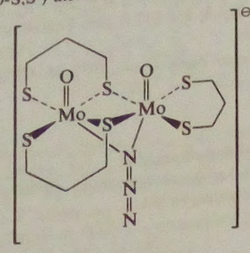
Bishop, M.W. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1 (*synth, pmr*)
Hursthouse, M.B. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1362 (*cryst struct*)
Minelli, M. *et al, Inorg. Chem.*, 1985, **24**, 1111 (*Mo-95 nmr, N-14 nmr*)

IC-006545

$C_9H_{18}Mo_2N_3O_2S_6^{\ominus}$

[μ-(Azido-N^1:N^1)]dioxobis[μ-[1,3-propanedithiolato(2−)-S:S,S']][1,3-propanedithiolato(2−)-S,S']dimolybdate(*VI*) (1−), 11CI

μ-Azido-N^1:N^1*-bis(μ-propane-1,3-dithiolato-*S:S,S′*)(propane-1,3-dithiolato-*S,S′*)-dioxodimolybdate*(VI)(*1*−)



M 584.5 (ion)
Non-linear azido group angle N-N-N 153.4°.

Ph_4P salt: [84535-99-9].
Dark red cryst. ($MeCN/Et_2O$).

Bishop, P.T. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 1052 (*cryst struct, synth*)

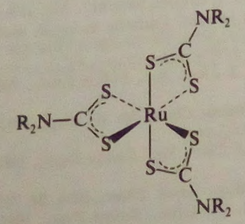
IC-006546

$C_9H_{18}N_3RuS_6$

Tris(*N*,*N*-dimethyldithiocarbamato)ruthenium(*III*)

*Tris(dimethylcarbamodithioato-*S,S′*)ruthenium*(III), *9CI*

[43190-67-6]



R = Me

M 461.7
Prepd. by treatment of $RuCl_3.xH_2O$ with $Na[S_2CNMe_2]$. Green cryst. Sol. polar solvs. Mp 293-294°. μ_{eff} = 1.77μ_B. Many other $Ru(S_2CNR_2)_3$ homologues are known.

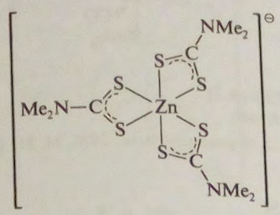
Malatesta, L., *Gazz. Chim. Ital.*, 1955, **85**, 1111 (*synth*)
DeSimone, R.E., *J. Am. Chem. Soc.*, 1973, **95**, 6238 (*esr*)
Raston, C.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 2405 (*synth, magnetism*)
Hendrickson, A.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2032 (*synth, uv, electrochem, magnetism, ir*)
Mattson, B.M. *et al*, *Inorg. Chem.*, 1977, **16**, 488 (*reactions*)
Given, K.W. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 4855 (*photochem*)
Given, K.W. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 1309 (*ms*)
Miessler, G.L. *et al*, *Inorg. Chem.*, 1979, **18**, 210 (*photochem*)
Ahmed, M. *et al*, *Proc. - Indian Acad. Sci., Sect. A*, 1979, **88**, 401 (*electrochem*)
Montree, A. *et al*, *Inorg. Chim. Acta*, 1987, **132**, 207 (*electrochem*)

$C_9H_{18}N_3S_6Zn^{\ominus}$

IC-006547

Tris(*N*,*N*-dimethyldithiocarbamato)zincate(1−)

*Tris(dimethylcarbamodithioato)zincate(*1−*).*
*Bis(dimethylcarbamodithioato-*S*)(dimethylcarbamodithioato-*S,S′*)zincate(*1−*), 9CI*



M 426.0 (ion)
6-Coord. anion in solid state with 4 short and 2 long Zn—S contacts.

Me_4N salt: [75642-17-0].
Cryst. (Me_2CO/pet. ether). Forms a monohydrate.
Et_4N salt: [61933-78-6].
Colourless needles (Me_2CO/pet. ether).
Tetrabutylammonium salt: [55913-65-0].
Cryst. (Me_2CO/pet. ether).

[55913-64-9, 62259-68-1]

Ashworth, C.C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1976, 743 (*cryst struct*)
McCleverty, J.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 2169; 1980, 1939, 1945 (*synth, ir, pmr, cryst struct*)

IC-006548

$C_9H_{18}N_4ORhS_6^{\oplus}$

Tris(*N*,*N*-dimethyldithiocarbamato)nitrosylrhodium(*III*) (1+)

*(Dimethylcarbamodithioato-*S*)bis(dimethylcarbamothioato-*S,S*)nitrosylrhodium(*1+*), 10CI*

$[Rh(NO)(S_2CNMe_2)_3]^{\oplus}$

M 493.5 (ion)
Geometry uncertain; may be 6- or 7-coordinate.

Hexafluorophosphate: [62793-28-6].
Brown solid.
Tetrafluoroborate: [62793-43-5].
Brown solid (CH_2Cl_2). Sol. CH_2Cl_2.

Connelly, N.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 70 (*synth, ir*)

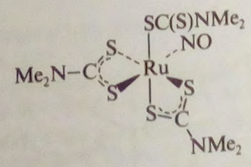
IC-006549

$C_9H_{18}N_4ORuS_6$

Tris(*N*,*N*-dimethyldithiocarbamato)(nitrosyl)ruthenium

*(Dimethylcarbamodithioato-*S*)bis(dimethylcarbamodithioato-*S,S′*)nitrosylruthenium, 9CI*

[51139-59-4]



M 491.7
Approx. octahedral complex. Contains both monodentate and bidentate dithiocarbamate, but is rigid on the pmr time scale. Prep. by treating $Ru(S_2CNMe_2)_3$ with NO. Red cryst. Mp 220-221°. Ir ν_{NO} 1830 cm^{-1}.

[54892-03-4]

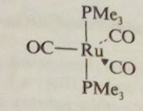
Cambi, L. *et al*, *Rend. Ist. Lomb. Accad. Sci. Lett., A*, 1938, **71**, 118 (*synth*)
Domenicano, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1966, 476 (*synth, ir*)
Johnson, B.F.G. *et al*, *J. Chem. Soc. A*, 1969, 1668 (*pmr*)
Miki, E. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 3779 (*ir*)
Su, C.-C. *et al*, *J. Organomet. Chem.*, 1975, **84**, 53 (*pe*)
Dubrawski, J.V. *et al*, *Inorg. Chem.*, 1980, **19**, 355 (*synth, pmr, ir*)

IC-006550

$C_9H_{18}O_3P_2Ru$

Tricarbonylbis(trimethylphosphine)ruthenium(0), 10CI

[75687-45-5]



M 337.2
Trigonal bipyramidal with axial P, Ru—P 234 pm. Prepd. by treating tri-μ-methylenehexakis(trimethylphosphine) diruthenium in toluene at 60° with CO (5 atm.). White cryst. (toluene). Sol. Me_2CO, C_6H_6. Ir ν_{CO} 1885 cm^{-1} (nujol).

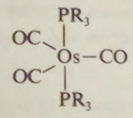
Jones, R.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1771 (*synth, ir, pmr, P-31 nmr, cryst struct*)

IC-006551

$C_9H_{18}O_9OsP_2$

Tricarbonylbis(trimethyl phosphite-*P*)osmium

Tricarbonylbis(phosphorous acid)osmium hexamethyl ester, 8CI



R = OMe

M 522.3
trans-form [22377-52-2]
Colourless cryst. (hexane). Mp 60°.

Bruce, M.I. *et al*, *J. Chem. Soc. A*, 1969, 987 (*synth, ir, pmr*)

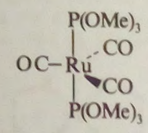
IC-006552

$C_9H_{18}O_9P_2Ru$

Tricarbonylbis(trimethyl phosphite-*P*)ruthenium

Tricarbonylbis(phosphorous acid)ruthenium hexamethyl ester, 8CI

[31541-94-3]



M 433.2
trans-form [30759-74-1]
Synth. from $Ru_3(CO)_{12}$ + $P(OMe)_3$ in hexane at r.t. White cryst. (hexane). Mp 54.5°. Ir ν_{CO} 1931, 1923 cm^{-1} (cyclohexane).

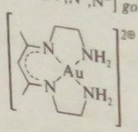
Burt, R. *et al*, *J. Chem. Soc. A*, 1969, 2645 (*reactions*)
Cooke, M. *et al*, *J. Chem. Soc. A*, 1971, 16 (*synth, ir, pmr, ms*)
Cobbledick, R.E. *et al*, *J. Organomet. Chem.*, 1980, **195**, 77 (*synth, ir*)
Graaf, J.L. *et al*, *Organometallics*, 1982, **1**, 837 (*synth, ir*)

IC-006553

$C_9H_{19}AuN_4^{2\oplus}$

[*N*,*N*′-Bis(aminoethyl)-2,4-pentanediiminato]gold(*III*) (2+)

[[N,N″-(1,3-Dimethyl-1,3-propanediylidene) bis[1,2-ethanediaminato]](1−)-N,N′,N″,N‴] gold(2+), 10CI



M 380.2 (ion)

Diiodide: [65681-96-1].
$C_9H_{19}AuI_2N_4$ M 634.0
Orange cryst. (EtOH). Mp 221-223°.
Bis-hexafluorophosphate: [71393-61-8].
Orange cryst. (EtOH).

Brawner, S.A. *et al*, *Inorg. Chem.*, 1978, **17**, 1304 (*synth, ir, pmr*)
Kim, J.H. *et al*, *Inorg. Chem.*, 1979, **18**, 3145 (*reactions*)

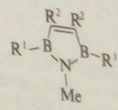
IC-006554

$C_9H_{19}B_2N$

3,4-Diethyl-2,5-dihydro-1,2,5-trimethyl-1*H*-1,2,5-azadiborole, 10CI

3,4-Diethyl-1,2,5-trimethyl-1,2,5-azadiborolene

[75532-24-0]



R¹ = Me, R² = CH_2CH_3

M 162.8
Forms transition-metal sandwich complexes such as Tricarbonyl[(3,4-η)-3,4-diethyl-2,5-dihydro-1,2,5-trimethyl-1*H*-1,2,5-azadiborole-B^2,B^5,N^1]iron, IC-007752, Bis[(3,4-η)-3,4-diethyl-2,5-dihydro-1,2,5-trimethyl-1*H*-1,2,5-azadiborole-B^2,B^5,N^1]nickel, IC-010076 and (η^5-2,4-Cyclopentadien-1-yl)[(3,4-η)-3,4-diethyl-2,5-dihydro-1,2,5-trimethyl-1*H*-1,2,5-azadiborole-B^2,B^5,N^1]cobalt, IC-008708. Liq., sensitive to air and moisture. Bp_{10} 80-82°.

Siebert, W. *et al*, *Z. Naturforsch., B*, 1980, **35**, 873 (*synth, props, ms, ir*)

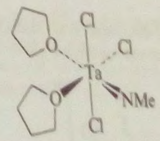
IC-006555

$C_9H_{19}Cl_3NO_2Ta$

Trichloro(methylimido)bis(tetrahydrofuran)tantalum(*V*)

Trichloro[methanaminato(2−)]bis(tetrahydrofuran) tantalum(V), *11CI*

[75730-61-9]



M 460.5
Octahedral. Synth. from $Ta(CHCMe_3)(THF)_2Cl_3$ and MeN=CHPh.

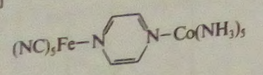
Rocklage, S.M. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 3077; 1980, **102**, 7808 (*synth, pmr*)

$C_9H_{19}CoFeN_{12}$ IC-006556

Pentakis(cyano-*C*)(pentaamminecobalt)[μ-(pyrazine-N^1,N^4)]iron, 10CI

Pentaamminecobalt(III)-μ-*pyrazole*(*pentacyano*)*ferrate*(II)

[66840-84-4]



M 410.1

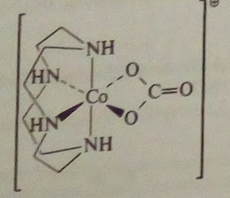
Prepd. in aq. soln., not isolated.

Malin, J.M. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 2097 (*synth, photochemistry, kinetics*)

$C_9H_{20}CoN_4O_3^{\oplus}$ IC-006557

[Carbonato(2−)-*O*-*O'*](1,4,7,10-tetraazacyclododecane-N^1,N^4,N^7,N^{10})cobalt(*III*)(1+), 9CI

[61475-39-6]



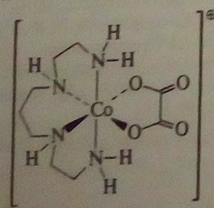
M 291.2 (ion)

Perchlorate: [61475-41-0].
Reddish violet cryst. + $1H_2O$ (aq. EtOH). Sol. H_2O.

Collman, J.P. *et al*, *Inorg. Chem.*, 1966, **5**, 1380 (*synth, uv*)
Loehlin, J.H. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 3063 (*cryst struct*)

$C_9H_{20}CoN_4O_4^{\oplus}$ IC-006558

Oxalato(1,4,8,11-tetraazaundecane)cobalt(*III*)(1+)



M 307.2 (ion)

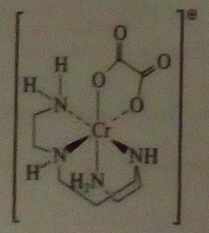
Oxalate, tetrahydrate: Red solid.

Bosnich, B., *J. Chem. Soc. A*, 1966, 1331 (*synth, uv*)

$C_9H_{20}CrN_4O_4^{\oplus}$ IC-006559

(1,9-Diamino-3,7-diazanonane)oxalatochromium(*III*)(1+)

Oxalato(*1,4,8,11-tetraazaundecane*)*chromium*(III)(*1+*)



cis,β-form

M 300.2 (ion)

Resolved and used to prepare racemic and chiral *cis*-derivs. e.g. (1,9-Diamino-3,7-diazanonane) bis(isothiocyanato)chromium(*III*)(1+), IC-006560.

cis-β-form

Bromide: Synth. from $Na_2Cr_2O_7$ + oxalic acid in H_2O, heat, add ligand then NaBr. Orange cryst. (aq. NaBr at 60°).

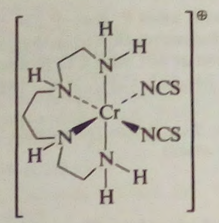
Perchlorate: Insol. H_2O.

House, D.A. *et al*, *Inorg. Chim. Acta*, 1983, **74**, 179 (*synth, uv-vis, resol, cd*)

$C_9H_{20}CrN_6S_2^{\oplus}$ IC-006560

(1,9-Diamino-3,7-diazanonane)bis(isothiocyanato) chromium(*III*)(1+)

[N,N'-*Bis*(*2-aminoethyl*)-*1,3-propanediamine*-N,N',N'',N''']*bis*(*thiocyanato*-N)*chromium*(III)(*1+*), *11CI*. (R,S)-(*1,4,8,11-Tetraazaundecane*)*bis*(*isothiocyanato*)*chromium*(III)



cis,α-form

M 328.4 (ion)

Octahedral cation.

cis, α-form

This isomer also known for other monodentate ligands.

Thiocyanate: Orange cryst. Sol. Me_2CO, MeOH. Also obt. in resolved form.

trans-form

Prepd. by a route expected to yield *cis*-form; Cr—NCS_{av} 198, Cr—N_{av} 207.1 pm.

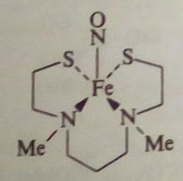
Thiocyanate: [81603-14-7].
Synth. from *cis*-[Cr(ligand)Cl_2]Cl.H_2O + NaSCN in H_2O. Orange red cryst. λ_{max} 232, 308, 362, 485 nm.

Macke, H.R. *et al*, *Inorg. Chem.*, 1982, **21**, 3080 (*cryst struct, trans-form, synth, uv-vis, ir*)
House, D.A. *et al*, *Inorg. Chim. Acta*, 1983, **74**, 179 (*synth, cis-form, resol, uv-vis*)

$C_9H_{20}FeN_3OS_2$ IC-006561

Nitrosyl[[2,2'-[1,3-propanediylbis(methylimino)]-bis[ethanethiolato]](2−)-*N*,*N'*,*S*,*S'*]iron, 10CI

[64175-41-3]



M 306.2

Square pyramidal at Fe. Prepd. from L_2Fe_2 + $(NO)PF_6$ or from L_2Fe_2 + NO in MeOH. Green cryst. Sol. CH_2Cl_2; insol. Et_2O; spar. sol. MeOH.

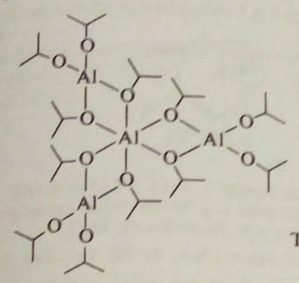
Karlin, K.D. *et al*, *Inorg. Chem.*, 1977, **16**, 3262 (*synth, uv, ir*)
Baltusis, L.M. *et al*, *Inorg. Chem.*, 1980, **19**, 2627 (*struct, deriv*)

$C_9H_{21}AlO_3$ IC-006562

Aluminum isopropoxide

2-Propanol aluminum salt, 9CI. Isopropyl alcohol aluminum salt, 8CI

[555-31-7]



Tetramer

M 204.2

Reagent for Meerwein-Ponndorf reactions, alcoholysis and ester exchange, synth. of higher alkoxides, chelates and acylates. Trimeric liq. which slowly solidifes to a tetrameric white solid. Mp 118°. Bp_5 145-150°.

▷ BD0975000.

Whitaker, G.C., *Adv. Chem. Ser.*, No. 23, 1959, 184 (*rev*)
Shiner, V.J. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 2318 (*struct, pmr*)
Daasch, L.W. *et al*, *Org. Mass Spectrom.*, 1969, **2**, 1043 (*ms*)
Fieggen, W. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1971, **90**, 410 (*ir, raman*)
Akitt, J.W. *et al*, *J. Magn. Reson.*, 1974, **15**, 162 (*nmr, struct*)
Turova, N.Ya. *et al*, *J. Inorg. Nucl. Chem.*, 1979, **41**, 5 (*cryst struct*)

$C_9H_{21}AsO_3$ IC-006563

Triisopropyl arsenite, 8CI

Tris(*1-methylethyl*) *arsenite, 9CI. Arsenous acid tris*(*1-methylethyl*) *ester, 9CI. Triisopropoxyarsine. Triisopropoxoarsenic. Tris*(*1-methylethoxo*)*arsenic*

[39936-83-9]

$As[OCH(CH_3)_2]_3$

M 252.1

Liq. Bp_{10} 58°.

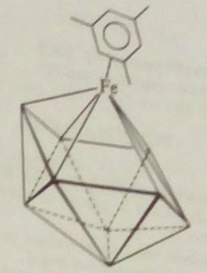
Brill, T.B. *et al*, *Inorg. Chem.*, 1973, **12**, 1884 (*synth, ir, nqr*)
Kober, F. *et al*, *Z. Anorg. Allg. Chem.*, 1973, **403**, 56 (*synth, pmr*)
Zakirov, D.U. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **235**, 1343; *Dokl. Phys. Chem.* (*Engl. Transl.*), 1977, **235**, 831 (*nqr*)
Baer, C.D. *et al*, *Inorg. Chem.*, 1983, **22**, 1402 (*reactions*)
Omiadze, A.P. *et al*, *Zh. Fiz. Khim.*, 1986, **60**, 1575; *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1986, **60**, 947 (*props*)

$C_9H_{21}B_9Fe$ IC-006564

[η⁶-Nonahydrononaborato(2−)][1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]iron, 11CI

1-(η⁶-*Mesitylene*)-*1-ferra*[C_3,-(1$v^6$3$v^4$3$v^5$3v^5)-Δ^{10}-*closo*]*decaborane*(9)

[92524-62-4]



M 282.4

closo-. Synth. from Fe vapour + $B_{10}H_{14}$ and mesitylene. Reddish-brown cryst. (C_6H_6/hexane by chromatog.). Sol. C_6H_6. Mp 236-237.5° dec.

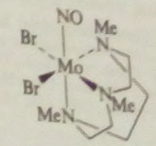
Micciche, R.P. *et al*, *Inorg. Chem.*, 1984, **23**, 3992 (*synth, ir, B-11 nmr, pmr, ms, struct*)

$C_9H_{21}Br_2MoN_4O$ IC-006565

Dibromonitrosyl(1,4,7-trimethyl-1,4,7-triazacyclononane-N^1,N^4,N^7)molybdenum

Dibromonitrosyl(*octahydro-1,4,7-trimethyl-1H-1,4,7-triazonine*-N^1,N^4,N^7)*molybdenum*, *11CI*

[98839-79-3]



M 457.0

Monomeric with disordered NO; proposed struct. shown. Metal centre in octahedral environment. Stable red-green dichroic cryst. (MeCN aq.). Forms green soln. in DMF, MeCN or MeOH and red soln. in aq. MeCN or aq. MeOH. Ir ν_{NO} 1565 cm^{-1} (KBr); μ_{eff} = 1.83μ_B (98-298K).

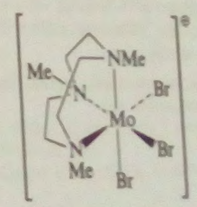
Backes-Daumann, G. *et al*, *Inorg. Chem.*, 1985, **24**, 4044 (*cryst struct, synth, ms, ir, electrochem, uv-vis*)

$C_9H_{21}Br_3MoN_3^{\oplus}$ IC-006566

Tribromo(1,4,7-trimethyl-1,4,7-triazacyclononane-N^1,N^4,N^7)molybdenum(*IV*)(1+)

Tribromo(*octahydro-1,4,7-trimethyl-1H-1,4,7-triazonine*-N^1,N^4,N^7)*molybdenum*(IV)(*1+*), *11CI*

[94370-67-9]



M 506.9 (ion)
pseudo-Octahedral cation.
Hexafluorophosphate: [94370-83-9].
Obt. by oxidation of $LMo(CO)_3$ with conc. HNO_3 at r.t. Red cryst. Sol. MeCN, DMSO; dec. in EtOH.

Backes-Dahmann, G. *et al*, *Inorg. Chem.*, 1985, **24**, 485 (*cryst struct, synth*)

IC-006567

$C_9H_{21}ClO_3Ti$
Chlorotripropoxytitanium(*IV*), 11Cl
Chlorotris(1-propanolato)titanium(IV)
[24287-11-4]

$TiCl(OCH_2CH_2CH_3)_3$

M 260.5
Tetrahedral. Synth. from $TiCl_4$ + $Ti(OCH_2CH_2CH_3)_4$ in pet. ether/C_6H_6. Used in manuf. of polyethylene and olefin copolymers.

Choukroun, R., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **278**, 113 (*synth, electrooptical props*)
Eur. Pat., 177 689, (1986); *CA*, **105**, 61097v (*use*)

IC-006568

$C_9H_{21}ClO_3Ti$
Chlorotris(2-propanolato)titanium(*IV*), 11Cl
Chlorotriisopropoxytitanium
[20717-86-6]

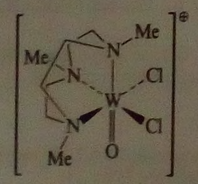
$TiCl[OCH(CH_3)_2]_3$

M 260.5
Tetrahedral. Synth. by adding $TiCl_4$ to $Ti(O^iPr)_4$ at 0° followed by distillation, or from $TiCl_4$, 2-propanol and Et_3N. Many patents cover the use of this compd. for olefin polym. Reacts like a Grignard reagent. Colourless solid. Sol. pentane, toluene, Et_2O, THF, CH_2Cl_2.

Choukroun, R. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **278**, 113 (*synth, magnetooptical props*)
Rausch, M.D. *et al*, *J. Organomet. Chem.*, 1974, **74**, 85 (*reactions*)
Czaja, K. *et al*, *Polimery (Warsaw)*, 1984, **29**, 411 (*use*)
Reetz, M.T. *et al*, *Chem. Ber.*, 1985, **118**, 1421 (*synth, reactions*)

IC-006569

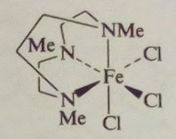
$C_9H_{21}Cl_2N_3OW^{\oplus}$
Dichlorooxo(*N,N',N''*-trimethyl-1,4,7-triazacyclononane-*N*^{1},*N*^{4},*N*^{7})tungsten(*V*)(1+)
Dichloro(octahydro-1,4,7-trimethyl-1H-1,4,7-triazonine-N^1,N^4,N^7*)oxotungsten*(V)(1+), *11Cl*



M 442.0 (ion)
Exhibits distortional isomerism; blue form W=O 172, green form 189 pm. Sol. MeCN. μ_{eff} = 1.90μ_B.
Hexafluorophosphate: [97879-02-2].
Blue or green cryst. (dimorph.). Blue form is hydrolytically stable.

Wieghardt, K. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 777 (*cryst struct, synth, uv-vis, esr*)

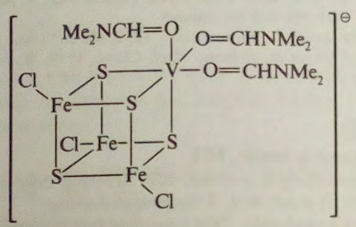
$C_9H_{21}Cl_3FeN_3$
IC-006570
Trichloro(1,4,7-trimethyl-1,4,7-triazacyclononane)iron(*III*)
Trichloro(octahydro-1,4,7-trimethyl-1H-1,4,7-triazonine-N^1,N^4,N^7*)iron*(III), *11Cl*
[110827-37-7]



M 333.4
Synth. from triaza ligand + $FeCl_3.6H_2O$ in EtOH. Precursor for protein (e.g. hemerythrin) model compds. Air-stable yellow ppt. Insol. EtOH, Et_2O.

Wieghardt, K. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1985, **24**, 392 (*synth, use*)
Hartman, J.A.R. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 7387 (*use*)
Chaudhuri, P. *et al*, *Prog. Inorg. Chem.*, 1987, **35**, 329 (*rev*)
Chaudhuri, P. *et al*, *Inorg. Chem.*, 1988, **27**, 1564 (*synth, use*)

$C_9H_{21}Cl_3Fe_3N_3O_3S_4V^{\ominus}$
IC-006571
Tris(*N,N*-dimethylformamide-*O*)tri-μ_3-thioxo(trichloro-μ_3-thioxotriferrate)vanadate(1−), 11Cl
Tris(dimethylformamide)tetra(μ_3-*sulfido*)*tris(chloroiron) vanadate*(1−)

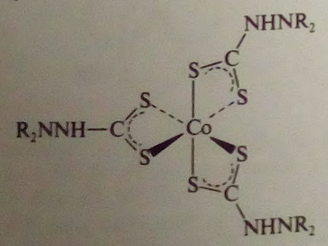


M 672.3 (ion)
The Mössbauer spectrum suggests a lower oxidation state than *IV* for vanadium. First example of an Fe—V cubane struct.
Me_4N salt: [99688-10-5].
Synth. from a slurry of $(NH_4)_3VS_4$, Me_4NBr and $FeCl_2$ in DMF. Black solid + 2DMF. Paramagnetic: μ_{eff} = 4.13μ_B (300K); 3.87 μ_B (8K).

Kovacs, J.A. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 341 (*synth, cryst struct, magnetism, uv-vis, mössbauer*)

IC-006572

$C_9H_{21}CoN_6S_6$
Tris(3,3-dimethyldithiocarbazato)cobalt(*III*), 8Cl
[34195-96-5]



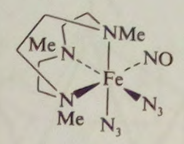
R = Me

M 464.6

Prob. struct. shown. Green solid.

Battistoni, C. *et al*, *Inorg. Nucl. Chem. Lett.*, 1971, **7**, 1081 (*synth, uv*)

$C_9H_{21}FeN_{10}O$
IC-006573
Diazidonitrosyl(1,4,7-trimethyl-1,4,7-triazacyclononane)iron
Diazidonitrosyl(octahydro-1,4,7-trimethyl-1H-1,4,7-triazonine-N^1,N^4,N^7*)iron*
[106633-07-2]



M 341.1
Octahedral; bent FeNO moiety. Synth. by adding NO to Tetraazidobis(1,4,7-trimethyl-1,4,7-triazacyclononane) diiron(*II*), IC-010105 in MeOH. Brown cryst. Sol. MeCN, MeOH, CH_2Cl_2. μ_{eff} = 4.06μ_B.

Pohl, K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1987, 187 (*synth, ir, struct, uv, magnetism*)
Chaudhuri, P. *et al*, *Prog. Inorg. Chem.*, 1987, **35**, 329 (*rev*)

$C_9H_{21}GaO_3$
IC-006574
Gallium(*III*) isopropoxide
Triisopropoxygallium. 2-Propanol gallium salt (3:1). Isopropanol gallium salt
[4452-61-3]

$Ga[OCH(CH_3)_2]_3$

M 246.9
Approx. dimer in C_6H_6. Synth. from $Ga(OEt)_3$ + 2-propanol. Starting material for a range of other alkoxides. Colourless viscous moisture-sensitive liq. Sol. C_6H_6. Bp_1 120°. Et, propyl, butyl and *tert*-butyl derivs. also descr.

Mehrotra, R.C. *et al*, *Curr. Sci.*, 1964, **33**, 241; *CA*, **60**, 15722 (*synth*)
Reinmann, R. *et al*, *Z. Naturforsch., B*, 1965, **20**, 524 (*synth*)
Bindal, S.R. *et al*, *Inorg. Chem.*, 1968, **7**, 384 (*reactions*)
Bindal, S.R. *et al*, *J. Chem. Soc. A*, 1969, 863 (*reactions*)

$C_9H_{21}N_3O_6PPd^{\ominus}$
IC-006575
Tris(nitrito-*N*)(tripropylphosphine)palladate(*II*)(1−)

$[Pd(NO_2)_3P[CH(CH_3)_2]_3]^{\ominus}$

M 404.6 (ion)
Square planar anion. Only isol. pure when large counter-ion present.
Ph_4As salt: [119823-50-6].
Yellow cryst. ($MeOH/Et_2O$). Sol. MeOH. V. long Pd—N bond *trans*- to phosphine.

Bruno, G. *et al*, *Polyhedron*, 1989, **8**, 161; 1990, **9**, 2591 (*synth, cryst struct*)

$C_9H_{21}O_3Sb$
IC-006576
Triisopropyl antimonite
Triisopropoxystibine. Antimonic acid (H_3SbO_3)*, triisopropyl ester, 9CI, 8CI. Tris(1-methylethyl) antimonite. Tris(1-methylethoxy)stibine. Triisopropoxoantimony. Tris(1-methylethoxo)antimony*
[18770-47-3]

$Sb[OCH(CH_3)_2]_3$

M 299.0
Liq. $Bp_{0.05}$ 29°.
Brill, T.B. *et al*, *Inorg. Chem.*, 1973, **12**, 1884 (*synth, ir, ms, nqr*)

$C_9H_{21}O_4V$
IC-006577
Oxotripropoxyvanadium(*V*), 11Cl
Vanadic acid tripropyl ester 9CI
[1686-23-3]

$VO(OCH_2CH_2CH_3)_3$

M 244.2
Tetrahedral (C_{3v}). Synth. from $VOCl_3$ and $PrSi(OPr)_3$ or from V_2O_5 and propanol in C_6H_6. Catalyses a v. wide range of reactions. Yellow liq. $Bp_{1.5}$ 97°.
Pascal, C. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1970, **271**, 1 (*magnetism, props*)
Lachowicz, A. *et al*, *Z. Anorg. Allg. Chem.*, 1975, **418**, 65 (*synth, pmr*)
Paulsen, K. *et al*, *Z. Naturforsch., A*, 1982, **37**, 139 (*V-51 nmr*)
U.S. Pat., 4 525 468, (1985); *CA*, **104**, 51248k (*use*)
Ger. Pat., 3 447 290, (1986); *CA*, **105**, 227023v (*synth*)

$C_9H_{21}O_6Y$
IC-006578
Tris(2-methoxyethanolato)yttrium(*III*)
[2172-12-5]

$Y(OCH_2CH_2OMe)_3$

M 314.1
Decameric.
Decamer:
$C_{90}H_{210}O_{60}Y_{10}$ M 3141.6
Used to synth. $YBa_2Cu_3O_7$. Air-sensitive cryst. V. sol. many org. solvs. 7-Coord.

Ravindranathan, P. *et al*, *J. Mater. Sci.*, 1988, **3**, 810 (*synth*)
Poncelet, O. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 1847 (*synth, ir, cryst struct*)
Poncelet, O. *et al*, *Inorg. Chem.*, 1990, **29**, 2883 (*reaction*)

$C_9H_{22}AlO_6^{\ominus}$
IC-006579
Hydrotris(2-methoxyethanolato)aluminate(1−)

$[AlH(OCH_2CH_2OMe)_3]^{\ominus}$

M 253.2 (ion)
Na salt: [28882-07-7].
Synth. from Sodium dihydrobis(2-methoxyethanolato-*O,O'*)aluminate(1−), IC-005251 + $MeOCH_2CH_2OH$ or from $NaAlH_4$ + $NaAl(OCH_2CH_2OMe)_4$. Selective reducing agent for ketones. Yellow syrupy moisture-sensitive liq.; usually made in C_6H_6 and used *in situ*. Sol. C_6H_6, ethers.

Časenský, B. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 2648 (*synth*)
Štrouf, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, **36**, 2707; 1974, **39**, 1044 (*synth, use*)
Kříž, O. *et al*, *Collect. Czech. Chem. Commun.*, 1973, **38**, 2076 (*analogues*)

IC-006580

$C_9H_{22}BO_3^{\ominus}$

Hydrotris(2-propanolato)borate(1−), 10CI, 9CI

Hydrotriisopropoxyborate. Triisopropoxyhydroborate. Triisopropoxyborohydride. Triisopropoxyhydridoborate

$[(H_3C)_2CHO]_3BH^{\ominus}$

M 189.0 (ion)

K salt: [42278-67-1]. *Feeble hydride*

$C_9H_{22}BKO_3$ M 228.1

Commercially available as THF soln. Catalyst for carbonylation of organoboranes. Mild reducing agent, comparable in props. to $NaBH_4$, but sol. in THF. Moisture-sensitive. Sol. THF.

▷ Flash pt. of THF soln. −15°.

Brown, C.A. *et al, J. Chem. Soc., Chem. Commun.*, 1973, 391 (*synth*)

Brown, H.C., *CA*, 1974, **80**, 37205y.

Brown, C.A. *et al, J. Am. Chem. Soc.*, 1979, **101**, 3964 (*props, use*)

Brown, H.C. *et al, Synthesis*, 1979, 701 (*use*)

Steinmetz, G.R. *et al, J. Am. Chem. Soc.*, 1981, **103**, 1278 (*use*)

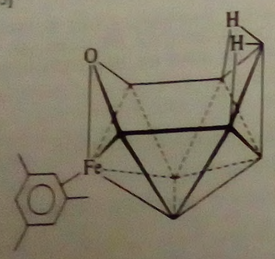
IC-006581

$C_9H_{22}B_9FeO$

[η⁴-Decahydrooxooctaborato(2−)-*O*][(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]iron, 11CI

8-(η⁶-Mesitylene)-(3,6-μH)(3,7-ηH)-2-oxa-8-ferra-1-deba[C_{2v}-(*1v⁶2v⁴4v¹2v⁵2v⁵*)-Δ^{18}-closo]*undecaborane(10)*

[92524-63-5]



M 288.6

Fe—O 194.2 pm. *nido*-. Synth. from Fe vapour + $B_{10}H_{14}$ + 1,3,5-trimethylbenzene. Yellow cryst. (C_6H_6/hexane by chromatog. in air).

Micciche, R.P. *et al, Inorg. Chem.*, 1984, **23**, 3992 (*synth, cryst struct, ms*)

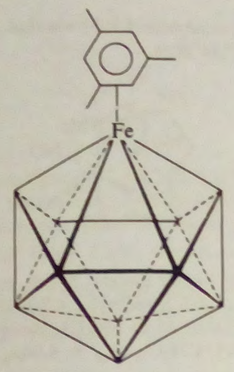
IC-006582

$C_9H_{22}B_{10}Fe$

[η⁶-Decahydrodecaborato(2−)][(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]iron, 11CI

1-(η⁶-Mesitylene)-1-ferra[C_{2v}-(*1v⁶2v⁴4v⁵2v⁵2v⁵*)-Δ^{18}-closo]*undecaborane(10)*

[92543-04-9]



M 294.2

closo-. Air-sensitive yellow cryst. (C_6H_6/hexane by chromatog.). Sol. C_6H_6.

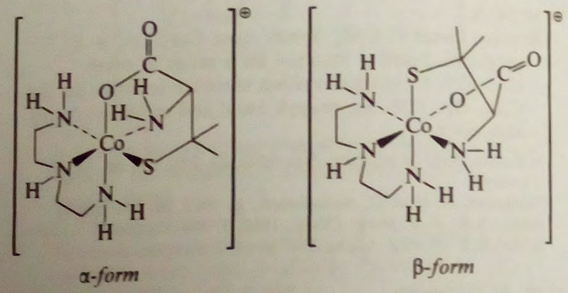
Micciche, R.P. *et al, Inorg. Chem.*, 1984, **23**, 3992 (*synth, ir, B-11 nmr, pmr, ms, struct*)

IC-006583

$C_9H_{22}CoN_4O_2S^{\oplus}$

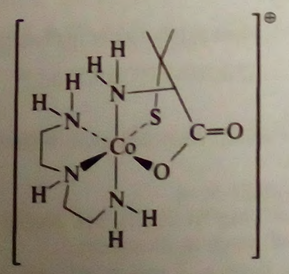
(Diethylenetriamine)(L-penicillaminato)cobalt(*III*)

[N-(*2-Aminoethyl*)-*1,2-ethanediamine*-N,N′,N‴][*3-mercapto-L-valinato*(2−)-N,O,S]*cobalt*(III)(1+), *11CI*



α-form

β-form



γ-form

M 309.2 (ion)

All three known isomers have *fac*-config. See also Bis(D-pencillaminato)cobaltate(*III*)(1−), IC-007003 and Bis(*S*-methyl-D-penicillaminato)cobalt(*III*), IC-007843.

α-form

Chloride: [86941-77-7].
Dark brown needles.

β-form

Chloride: [86941-78-8].

Dark brown needles.

γ-form

Chloride: [86941-79-9].
Dark brown needles.

Wakayama, K. *et al, Bull. Chem. Soc. Jpn.*, 1982, **55**, 3473; 1983, **56**, 1995 (*synth, struct, cd*)

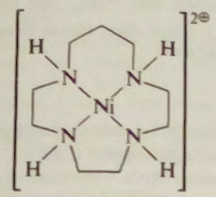
IC-006584

$C_9H_{22}N_4Ni^{2\oplus}$

(1,4,7,10-Tetraazacyclotridecane)nickel(*II*)(2+), 10CI

([13]AneN₄)nickel(2+)

[53277-10-4]



M 244.9 (ion)

Aqueous solns. show equilibrium with diaqua-adduct.

Diperchlorate: [71901-50-3].
$C_9H_{22}Cl_2N_4NiO_8$ M 443.8
Orange cryst. or yellow needles. Sol. H_2O, $MeNO_2$, MeOH.

Fabbrizzi, L., *J. Chem. Soc., Dalton Trans.*, 1979, 1857 (*synth, ir*)

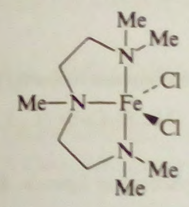
Coates, J.H. *et al, Aust. J. Chem.*, 1982, **35**, 903 (*synth, ir, magnetism*)

IC-006585

$C_9H_{23}Cl_2FeN_3$

Dichloro(*N,N,N′,N″,N‴*-pentamethyldiethylenetriamine)iron(*II*)

Dichloro[N-[*2-(dimethylamino)ethyl*]-N,N′,N′-*trimethyl-1,2-ethanediamine*-N,N′,N″]*iron*



M 300.0

Trigonal bipyramidal Fe. Synth. from $FeCl_2$ + ligand in 1-butanol. First example of a high spin 5-coord. Fe(*II*) complex. Amethyst-coloured cryst. ($CHCl_3$/pet. ether). Sol. $CHCl_3$.

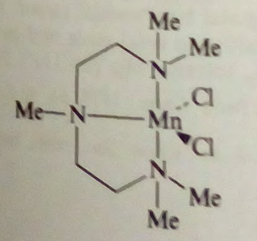
Ciampolini, M. *et al, Inorg. Chem.*, 1966, **5**, 45 (*synth, magnetism, str*)

IC-006586

$C_9H_{23}Cl_2MnN_3$

Dichloro(*N,N,N′,N″,N‴*-pentamethyldiethylenetriamine)manganese(*II*), 8CI

[16060-05-2]



M 299.1

High spin manganese(*II*) complex. μ_{eff} = 5.85μ_B (295K). Struct. assumed to be intermed. between trigonal- and bipyramidal square-pyramidal. Synth. by mixing hot solns. of $MnCl_2$ and a sl. excess of the triamine in 1-butanol. Hygroscopic white cryst. ($CHCl_3$/pet. ether); fairly stable in dry air. V. sol. ROH, $EtNO_2$, $PhNO_2$ and $CHCl_3$. Non-conductor in $CHCl_3$ and $PhNO_2$.

Ciampolini, M. *et al, Coord. Chem. Rev.*, 1966, **1**, 222 (*props*)

Ciampolini, M. *et al, Inorg. Chem.*, 1966, **5**, 45 (*synth, magnetism, reflectance spectrum, elect cond, struct*)

Paoletti, P., *Inorg. Chem.*, 1967, **6**, 64 (*thermodynamic data*)

Bryson, D. *et al, Spectrochim. Acta, Part A*, 1970, **26**, 2275 (*far ir*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, D3, 55 (*rev, bibl*)

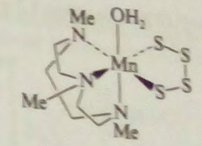
$C_9H_{23}MnN_3OS_4$

IC-006587

Aqua(tetrasulfido-*S*¹,*S*⁴)(*N,N′,N″*-trimethyl-1,4,7-triazacyclononane-*N,N′,N″*)manganese(*II*)

Aqua(*octahydro-1,4,7-trimethyl-1H-1,4,7-triazonine-N¹,N⁴,N⁷*)(*tetrathio*)*manganese*(II), *12CI*

[107760-74-7]



M 372.5

Synth. from $Mn(OAc)_2.2H_2O$ and *N,N′,N″*-trimethyl-1,4,7-triazacyclononane in MeOH under Ar and aq. $(NH_4)_2S$. Pale yellow cryst. (EtOH). μ_{eff} = 5.82μ_B.

Wieghardt, K. *et al, Inorg. Chim. Acta*, 1987, **126**, 39 (*synth, cryst struct, magnetism*)

IC-006588

$C_9H_{24}Br_2MnN_6O_3$

Dibromotris(*N,N′*-dimethylurea)manganese(*II*), 11CI

Manganese(II) *bromide tris*(N,N′-*dimethylurea*)

[75657-77-1]

$MnBr_2[O{=}C(NHMe)_2]_3$

M 479.0

Trigonal bipyramidal with equatorial Br. Prepd. by refluxing $MnBr_2.4H_2O$, N,N′-dimethylurea and 2,2′-dimethoxypropane in dry EtOH. Pink cryst. (EtOH/1-butanol 1:1); v. moisture-sensitive. Mp 202°. Corresp. chloride and iodide also known.

Barbier, J.-P. *et al, J. Inorg. Nucl. Chem.*, 1973, **35**, 781, 3026 (*synth, ir*)

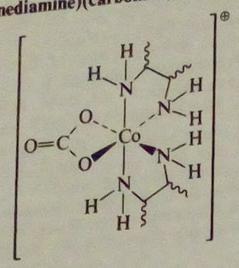
Barbier, J.-P. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1976, **95**, 213 (*ir*)

Delaunay, J. *et al, Inorg. Chem.*, 1986, **25**, 3957 (*cryst struct, ir*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, D5, 150 (*rev, bibl*)

IC-006589

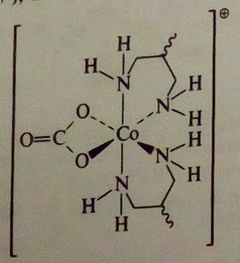
$C_9H_{24}CoN_4O_3^{\oplus}$
Bis(2,3-butanediamine)(carbonato)cobalt(*III*)(1+)



M 295.2 (ion)
Octahedral.
Iodide: [86852-57-5].
Red cryst. + $1H_2O$. Sol. H_2O.
Gargello, M.F. *et al, Inorg. Chem.*, 1983, **22**, 2888 (*synth, ir, cmr, cryst struct*)

IC-006590

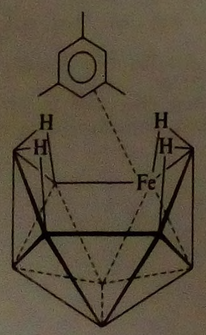
$C_9H_{24}CoN_4O_3^{\oplus}$
[Carbonato(2−)-*O,O'*]bis(2-methyl-1,3-propanediamine) cobalt(*III*)(1+), 1ICl



M 295.2 (ion)
Chloride: [86823-48-5].
Red solid. Sol. H_2O.
Gargello, M.F. *et al, Inorg. Chem.*, 1983, **22**, 2888 (*synth, cmr*)

IC-006591

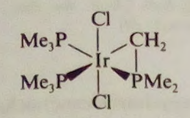
$C_9H_{25}B_9Fe$
[η^4-Tridecahydrononaborato(2−)][(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]iron, 1ICl
5-(η^6-Mesitylene)(2,4-μH)(2,5-μH)(3,6-μH)(3,7-μH)-5-ferra-1-debor[C_{2v}-(1$v^6$2$v^4$4$v^5$2$v^5$2v^5)-Δ^{18}-closo]*undecaborane(13)*
[92524-61-3]



M 286.4
Reddish-purple solid (C_6H_6/hexane by chromatog.). Sol. C_6H_6. Mp 175° dec.
Micciche, R.P. *et al, Inorg. Chem.*, 1984, **23**, 3992 (*synth, ir, ms, B-11 nmr, pmr, cryst struct*)

IC-006592

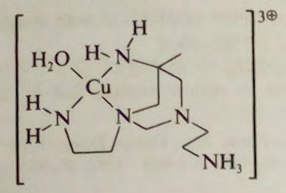
$C_9H_{26}Cl_2IrP_3$
Dichloro[(dimethylphosphino)methyl-*C,P*] bis(trimethylphosphine)iridium(*III*)
[79469-84-4]



M 490.3
Cyclometallated deriv. of PMe_3. Approx. octahedral.
Bright yellow cryst. Sol. C_6H_6. Mp 139-140°.
Al-Jibori, S. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1572 (*synth, ir, pmr, cmr, P-31 nmr*)

IC-006593

$C_9H_{26}CuN_5O^{3\oplus}$
(5-Amino-3-aminoethyl-1-ammonioethyl-5-methyl-1,3-diazacyclohexane)aquacopper(*II*)(3+)
Aqua[1,3-bis(2-aminoethyl)-5-ammonio-5-methyl-1,3-diazacyclohexane]copper(II)(3+) (*incorr.*)



M 283.8 (ion)
Cu has pseudo-square planar geometry.
Triperchlorate: [104198-62-1].
Blue plates. Insol. EtOH.
▷ Potentially explosive.
Comba, P. *et al, Inorg. Chem.*, 1986, **25**, 4260 (*synth, cryst struct, ir, uv, esr, electrochem*)

IC-006594

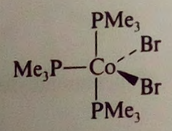
$C_9H_{27}BrCoP_3$
Bromotris(trimethylphosphine)cobalt(*I*), 9Cl

$(Me_3P)_3CoBr$ (C_{3v})

M 367.0
Co(*I*) stabilised by phosphine ligands. Blue cryst. Dec. >140°.
Klein, H.F. *et al, Inorg. Chem.*, 1975, **14**, 473 (*synth, ir*)

IC-006595

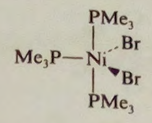
$C_9H_{27}Br_2CoP_3$
Dibromotris(trimethylphosphine)cobalt(*II*), 10Cl
[52810-40-9]



M 446.9
Esr suggests trigonal bipyramidal struct. Dark blue violet cryst.; air-sensitive in solid state and in soln. Sol. CH_2Cl_2, C_6H_6, toluene. Mp 109-111°. Paramagnetic.
Bressan, M. *et al, Inorg. Chem.*, 1975, **14**, 38 (*synth, uv, magnetism*)
Drago, R.S. *et al, J. Am. Chem. Soc.*, 1980, **102**, 1884 (*synth, esr*)

IC-006596

$C_9H_{27}Br_2NiP_3$
Dibromotris(trimethylphosphine)nickel(*II*), 9Cl
[53188-33-3]



M 446.7
Trigonal bipyramidal geometry. Blue-black cryst. (EtOH). Sol. C_6H_6, EtOH, CH_2Cl_2, Me_2CO. Mp 145-150° dec.
[20663-84-7, 21385-46-6]
Dahl, O., *Acta Chem. Scand.*, 1969, **23**, 2342 (*synth, ir, uv*)
Dawson, J.W. *et al, J. Am. Chem. Soc.*, 1974, **96**, 4428 (*cryst struct*)
Dartiguenave, M. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 2253 (*pmr*)
Meier, P.F. *et al, Inorg. Chem.*, 1979, **18**, 610 (*P-31 nmr*)

IC-006597

$C_9H_{27}Br_3IrP_3$
Tribromotris(trimethylphosphine)iridium(*III*), 9Cl

$IrBr_3(PMe_3)_3$

M 660.1
Octahedral geometry.
fac-form [42593-83-9]
White solid. Sol. $MeNO_2$. Mp 358°.
mer-form [42750-84-5]
Orange solid. Sol. CH_2Cl_2, $MeNO_2$.
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1489 (*synth, ir, raman*)

IC-006598

$C_9H_{27}Br_3P_3Rh$
Tribromotris(trimethylphosphine)rhodium(*III*), 9Cl
Rhodium(III) *bromide tris(trimethylphosphine)*
[42750-82-3]

$RhBr_3(PMe_3)_3$

M 570.8
mer-Octahedral. Yellow solid. Sol. $MeNO_2$. Dec. at 325°.
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1489 (*synth, ir, raman*)

IC-006599

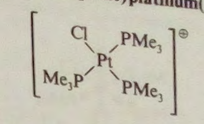
$C_9H_{27}ClCoP_3$
Chlorotris(trimethylphosphine)cobalt(*I*), 9Cl
[55516-89-7]

$Co(PMe_3)_3Cl$

M 322.6
Probably tetrahedral struct. Blue solid. Sol. pentane. Paramagnetic, dec. above 90°.
Klein, H.F. *et al, Inorg. Chem.*, 1975, **14**, 473 (*synth, ir, magnetism*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **3**, 2009 (*synth*)

IC-006600

$C_9H_{27}ClP_3Pt^{\oplus}$
Chlorotris(trimethylphosphine)platinum(*II*)(1+), 8Cl



M 458.7 (ion)
Square planar struct. with Pt—P bond longer when *trans* to Cl.
Chloride: [72778-75-7].
White cryst. Sol. CH_2Cl_2.
Nitrate: [28570-01-6].
Props not recorded. Sol. CH_2Cl_2.
Tetrafluoroborate: [21556-13-8].
Sol. H_2O, Me_2CO, CH_2Cl_2.
Duddell, D.A. *et al, J. Chem. Soc. A*, 1970, 545 (*synth, ir, raman*)
Goggin, P.L. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2220 (*pmr*)
Favez, R. *et al, Inorg. Chem.*, 1980, **19**, 1356 (*synth, struct, ir, uv, P-31 nmr*)

IC-006601

$C_9H_{27}ClP_3Rh$
Chlorotris(trimethylphosphine)rhodium, 11Cl, 10Cl
Rhodium(I) *chloride tris(trimethylphosphine)*
[36103-64-7]

$Rh(PMe_3)_3Cl$

M 366.5
Reports earlier than 1980 may be spurious. Probably square planar struct. Catalyses isomerisation of epoxides to ketones. Orange prisms (toluene at −20°). Sol. C_6H_6. Mp 205-210°. Slowly abstracts CO from ROH to give Carbonylchlorobis(trimethylphosphine)rhodium, IC-005794. Oxidatively adds R^{1}CHO to give RhH(COR^1)$(PMe_3)_3Cl$.
Intille, G.M. *et al, Inorg. Chem.*, 1972, **11**, 695 (*synth*)
Jones, R.A. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 511; 1981, 126 (*synth, cryst struct, pmr, P-31 nmr, props*)
Milstein, D., *J. Am. Chem. Soc.*, 1982, **104**, 5227 (*props*)
Milstein, D., *J. Chem. Soc., Chem. Commun.*, 1982, 1357 (*props*)
Milstein, D., *Organometallics*, 1982, **1**, 1549 (*props*)
Chandrasekhar, K. *et al, J. Am. Chem. Soc.*, 1983, **105**, 7081 (*struct*)

IC-006602

$C_9H_{27}Cl_2NiP_3$
Dichlorotris(trimethylphosphine)nickel(*II*), 9Cl
[37175-97-6]

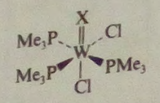
$NiCl_2(PMe_3)_3$

M 357.8
Prob. trigonal bipyramidal with eq. Cl. Dark blue powder. Sol. CH_2Cl_2. Mp 119-121° dec. Loses PMe_3 readily at r.t.
[53177-14-3]
Dawson, J.W. *et al, J. Am. Chem. Soc.*, 1974, **96**, 4428 (*synth, uv-vis*)

$C_9H_{27}Cl_2OP_3W$ IC-006603

Dichlorooxotris(trimethylphosphine)tungsten(*IV*), 11Cl

[87737-49-3]



X = O

M 498.9

mer-Octahedral. W=O 167 pm. Synth. from $WCl_4(PMe_3)_3$ + MeOH or H_2O in THF. Purple cryst. (Et_2O). Mp 134-135°. Ir $\nu_{W=O}$ 950 cm^{-1}.

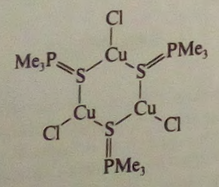
Carmona, E. *et al*, *Polyhedron*, 1983, **2**, 797 (*synth, ir, pmr*)
Chiu, K.W. *et al*, *Polyhedron*, 1983, **2**, 803 (*cryst struct, synth, P-31 nmr, pmr, ir*)
Carmona, E. *et al*, *Inorg. Chem.*, 1986, **25**, 3804 (*reactions*)

$C_9H_{27}Cl_3Cu_3P_3S_3$ IC-006604

Trichlorotris-μ-(trimethylphosphine sulfide-*S:S*)tricopper, 9Cl

(*Trimethylphosphine sulfide*)*chlorocopper*(I) *trimer*

[38656-77-8]



M 621.4

$SPMe_3$ bridges copper atoms in preference to chloride. Colourless cryst. (MeCN). Fairly insol. org. solvs.

Monomer:
$C_3H_9ClCuPS$ M 207.1

Tiethof, J.A. *et al*, *Inorg. Chem.*, 1973, **12**, 1170; 1974, **13**, 2505 (*cryst struct, synth*)
Kincaid, J. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 2091 (*ir*)
Bowmaker, G.A. *et al*, *Aust. J. Chem.*, 1975, **28**, 1431 (*ir, raman, nqr*)

$C_9H_{27}Cl_3IrP_3$ IC-006605

Trichlorotris(trimethylphosphine)iridium(*III*), 9Cl

$IrCl_3(PMe_3)_3$

M 526.8

fac-form [36385-77-0]
White solid. Sol. $MeNO_2$. Mp 363°.

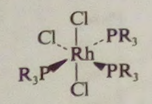
mer-form [36385-96-3]
$C_9H_{27}Cl_3IrP_3$ M 526.8
Yellow solid. Sol. CH_2Cl_2. Mp 295°.

Goggin, P.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1489 (*synth, ir, raman*)

$C_9H_{27}Cl_3P_3Rh$ IC-006606

Trichlorotris(trimethylphosphine)rhodium(*III*), 8Cl

Rhodium(III) *chloride tris*(*trimethylphosphine*)



mer-form

R = Me

M 437.4

Octahedral.

fac-form [36103-61-4]
Yellow-orange cryst. Sol. $CHCl_3$. Mp 160-170°.

mer-form [30185-45-6]
Orange cryst. Sol. C_6H_6. Mp 200-210°.

Grim, S.O. *et al*, *Inorg. Chim. Acta*, 1970, **4**, 277 (*synth, P-31 nmr, pmr*)
Intille, G.M. *et al*, *Inorg. Chem.*, 1972, **11**, 695 (*synth, pmr*)

$C_9H_{27}Cl_4N_3Th$ IC-006607

Tetrachlorotris(trimethylamine)thorium(*IV*)

[90479-84-8]

$(Me_3N)_3ThCl_4$

M 551.1

7-Coordinate with capped octahedral geometry. Air-sensitive colourless hexagonal cryst. Sol. C_6H_6, $CHCl_3$, Me_3N.

Drew, M.G.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 727 (*synth, cryst struct, ir, pmr*)

$C_9H_{27}Cl_4NbP_3$ IC-006608

Tetrachlorotris(trimethylphosphine)niobium(*IV*), 11Cl

Niobium(IV) *chloride tris*(*trimethylphosphine*)

[99350-61-5]

$NbCl_4(PMe_3)_3$

M 462.9

Synth. from Tetrachlorobis(tetrahydrofuran)niobium(*IV*), IC-006085 and Me_3P in toluene. Green solid. Sol. toluene.

Cotton, F.A. *et al*, *Polyhedron*, 1985, **4**, 1103 (*synth, cryst struct, esr*)

$C_9H_{27}Cl_4O_3P_3Th$ IC-006609

Tetrachlorotris(trimethylphosphine oxide)thorium(*IV*)

Thorium(IV) *chloride tris*(*trimethylphosphine oxide*)

[58057-88-8]

$ThCl_4(O{=}PMe_3)_3$

M 650.0

White solid. Sl. sol. THF. Mp 87° dec.

Wassef, M.A., *Indian J. Chem.*, 1975, **13**, 1205 (*synth, ir*)

$C_9H_{27}Cl_4O_3P_3U$ IC-006610

Tetrachlorotris(trimethylphosphine oxide)uranium(*IV*)

[41016-02-8]

$UCl_4(O{=}PMe_3)_3$

M 656.0

Blue-green solid (THF). Mp 95° dec.

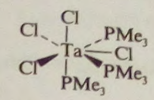
Gans, P. *et al*, *J. Chem. Soc.*, 1964, 4172 (*synth*)
Al-Kazzaz, Z.M.S. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1493 (*synth, ir*)

$C_9H_{27}Cl_4P_3Ta$ IC-006611

Tetrachlorotris(trimethylphosphine)tantalum(*IV*), 11Cl

Tantalum(IV) *chloride tris*(*trimethylphosphine*)

[92763-09-2]



M 550.9

Monocapped octahedron: Cl is the capping atom. Synth. from Tetrachlorobis(dimethylphenylphosphine) tantalum(*IV*), IC-009358 and Me_3P in CH_2Cl_2. Dark red solid.

Cotton, F.A. *et al*, *Inorg. Chem.*, 1984, **23**, 4046 (*synth, cryst struct*)

$C_9H_{27}Cl_4P_3U$ IC-006612

Tetrachlorotris(trimethylphosphine)uranium(*IV*)

[80290-56-8]

$(Me_3P)_3UCl_4$

M 608.0

Green cryst. Sol. PMe_3. Tends to lose PMe_3 on recryst. from other solvs.

Edwards, P.G. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 7792 (*synth*)

$C_9H_{27}CoIP_3$ IC-006613

Iodotris(trimethylphosphine)cobalt(*I*), 9Cl

[53432-08-9]

$Co(PMe_3)_3I$

M 414.0

Probably tetrahedral struct. Violet blue cryst. Sol. pentane. Paramagnetic, dec. above 114°.

Klein, H.F. *et al*, *Inorg. Chem.*, 1975, **14**, 473 (*synth, ir, magnetism*)

$C_9H_{27}CoN_2P_3^{\ominus}$ IC-006614

(Dinitrogen)tris(trimethylphosphine)cobaltate(1−), 11Cl

$[Co(N_2)(PMe_3)_3]^{\ominus}$

M 315.1 (ion)

Tetrahedral struct. with monodentate N_2.

▷Stable to 140° under N_2 but immediately ignites on exp. to air.

Li salt: [108009-03-6].
$C_9H_{27}CoLiN_2P_3$ M 322.1
Orange cryst. (THF at −78°). Sol. THF. Ir ν_{NN} 1735vs,br, 1715vs cm^{-1} (nujol). Dec. >142°.

Na salt: [108009-02-5].
Orange cryst. (Et_2O). Sol. Et_2O, THF. Ir ν_{NN} 1850m, 1770vs cm^{-1} (nujol).

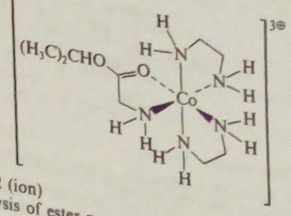
K salt: [63181-09-9].
Orange air-sensitive cryst. (Et_2O at −78°). Sol. Et_2O, THF. Ir ν_{NN} 1795vs,br, 1753m cm^{-1} (nujol).

Hammer, R.E., *Angew. Chem., Int. Ed. Engl.*, 1977, **18**, 485 (*synth, ir, cryst struct, props*)
Klein, H.F. *et al*, *Z. Naturforsch., B*, 1978, **33**, 1267 (*synth, struct*)
Klein, H.F. *et al*, *Organometallics*, 1987, **6**, 1341 (*synth, ir, props*)

$C_9H_{27}CoN_5O_2^{3\oplus}$ IC-006615

Bis(ethylenediamine)(isopropyl glycinate)cobalt(*III*)(3+)

Bis(*1,2-ethanediamine-N,N′*)(*1-methylethyl glycinate-N,O*)*cobalt*(III)(3+), 9Cl



M 296.2 (ion)

Hydrolysis of ester proceeds without rupture of chelate ring.

Triperchlorate: [29999-57-3].
Orange solid. Sol. DMSO, Me_2CO/MeOH.

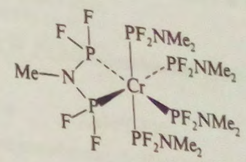
Buckingham, D.A. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 6032; 1970, **92**, 5571; 1972, **94**, 4032; 1973, **95**, 4173 (*synth, hydrol, reactions*)
Boreham, C.J. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 1409 (*reactions*)

$C_9H_{27}CrF_{12}N_5P_6$ IC-006616

[*N*-Methylaminobis(difluorophosphine)-*P,P′*]tetrakis(*N,N*-dimethylaminodifluorophosphine-*P*)chromium(0)

Tetrakis(*dimethylphosphoramidous difluoride-P*)(*methylimidodiphosphorous tetrafluoride-P,P′*)*chromium*, 11Cl, 10Cl

[68474-95-3]



M 671.1

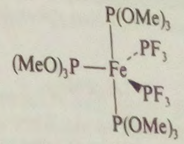
Distorted octahedral config. through small bite bidentate ligand. Stable, sublimable white cryst. (CH_2Cl_2).

King, R.B. *et al*, *Inorg. Chem.*, 1979, **18**, 364 (*synth*)
King, R.B. *et al*, *J. Organomet. Chem.*, 1985, **296**, 15 (*cryst struct*)

$C_9H_{27}F_6FeO_9P_5$ IC-006617

Bis(phosphorous trifluoride)tris(trimethyl phosphite-*P*)iron

[55086-71-0]



M 604.0

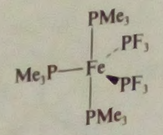
Synth. from $Fe[P(OMe)_3]_5$ + PF_3. Colourless. $^1J_{PF}$ 1213 Hz.

Muetterties, E.L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1974, 850 (*synth, nmr*)
Nixon, J.F., *Adv. Inorg. Chem. Radiochem.*, 1985, **29**, 41 (*rev*)

$C_9H_{27}F_6FeP_5$ IC-006618

Bis(phosphorous trifluoride)tris(trimethylphosphine) iron(0), 9CI

[56344-16-2]



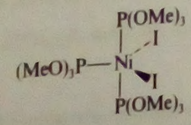
M 460.0
Trigonal bipyramidal. Yellow.

Muetterties, E.L. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 850 (*proposed struct, phosphite analogue*)
Rathke, J.N. *et al, J. Am. Chem. Soc.*, 1975, **97**, 3272 (*nmr*)
Nixon, J.F., *Adv. Inorg. Chem. Radiochem.*, 1985, **29**, 41 (*rev*)

$C_9H_{27}I_2NiO_9P_3$ IC-006619

Diiodotris(trimethyl phosphite-*P*)nickel(*II*), 9CI

[53966-17-9]



M 684.7
Nearly trigonal geometry around Ni. Discrete molecules. Air-sensitive dark-purple prisms (hexane).

Van de Griend, L.J. *et al, Inorg. Chem.*, 1975, **14**, 710 (*cryst struct*)
Bart, J.C.J. *et al, Phosphorus Sulfur*, 1983, **17**, 205 (*conform*)

$C_9H_{27}I_2NiP_3$ IC-006620

Diiodotris(trimethylphosphine)nickel(*II*), 9CI

[20663-85-8]

$NiI_2(PMe_3)_3$

M 540.7
Trigonal bipyramidal with eq. I. Green-black cryst. Sol. CH_2Cl_2. $\mu_{eff} = 0.58\mu_B$. Stable to dissociation; 2:1 complex not obt. Dec. at 165-170°.

[53188-34-4]

Dahl, O., *Acta Chem. Scand., Ser. C*, 1969, **23**, 2342 (*synth, uv-vis*)
Dawson, J.W. *et al, J. Am. Chem. Soc.*, 1974, **96**, 4428 (*uv-vis, magnetism*)
Meier, P. *et al, J. Am. Chem. Soc.*, 1976, **98**, 6402 (*P-31 nmr*)

$C_9H_{27}I_3P_3Ta$ IC-006621

Triiodotris(trimethylphosphine)tantalum(*III*), 11CI

Tantalum(III) *iodide tris(trimethylphosphine)*

[86024-26-2]

$TaI_3(PMe_3)_3$

M 789.8
Octahedral. Synth. from $Ta(C_2H_4)(PMe_3)I_3$ and PMe_3 in toluene. Brown-black solid. Sol. THF.

Turner, H.W. *et al, J. Am. Chem. Soc.*, 1983, **105**, 4942 (*synth, pmr*)

$C_9H_{27}NNiOP_3^{\oplus}$ IC-006622

Nitrosyltris(trimethylphosphine)nickel(1+), 11CI

$[Ni(NO)(PMe_3)_3]^{\oplus}$ (C_{3v})

M 316.9 (ion)
Hexafluorophosphate: [91924-79-7].
Violet air-sensitive cryst. (CH_2Cl_2/Et_2O). Ir ν_{NO} 1750 cm^{-1}. Paramagnetic, $\mu_{eff} = 0.99\mu_B$.

Elbaze, G. *et al, Inorg. Chim. Acta*, 1984, **87**, 91 (*synth, uv, ir, P-31 nmr, conductivity, cryststruct*)

$C_9H_{27}N_4NpO_{15}P_3$ IC-006623

Tetrakis(nitrato)tris(trimethylphosphine oxide-*O*) neptunium(*IV*)

[52580-38-8]

$Np(NO_3)_4(O{=}PMe_3)_3$

M 761.2
Dark green solid (EtOH). Sol. EtOH, $MeNO_2$, $CHCl_3$. Mp 188-189° dec. Possibly has both monodentate and bidentate nitrate.

Bagnall, K.W. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 889 (*synth, ir*)

$C_9H_{27}O_4Si_3V$ IC-006624

Oxotris(trimethylsilanolato)vanadium(*V*), 11CI

Vanadic acid tris(trimethylsilyl) ester

[5590-56-7]

$VO(OSiMe_3)_3$

M 334.5
Tetrahedral at V. Synth. either by reaction of Me_3SiCl with Ag_3VO_4 in CH_2Cl_2 at 10° or V_2O_5 with $Me_3SiOSiMe_3$ at 100°. A number of reactions, including rearrangement of unsatd. alcohols and synth. of substituted vitamin A have been patented. Colourless, easily hydrol. liq. Mp −18°. $Bp_{9.5}$ 100°, $Bp_{0.001}$ 48°.

Schmidt, M. *et al, Angew. Chem.*, 1959, **71**, 220 (*synth*)
U.S. Pat., 4 022 807, (1977); *CA*, **87**, 117976k (*Vitamin A derivs*)
Swiss Pat., 605 524, (1978); *CA*, **90**, 54564p (*use*)
Preuss, F. *et al, Z. Naturforsch., B*, 1981, **36**, 1130 (*synth*)

$C_9H_{27}P_3Rh^{\oplus}$ IC-006625

Tris(trimethylphosphine)rhodium(1+), 10CI

$[Rh(PMe_3)_3]^{\oplus}$

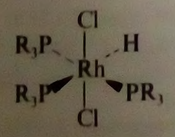
M 331.1 (ion)
Chloride: see *Chlorotris(trimethylphosphine)rhodium, IC-006601*
Hexafluorophosphate: [73969-98-9].
$C_9H_{27}F_6P_4Rh$ M 476.1
Yellow powder. Sol. $MeNO_2$; insol. H_2O, THF. Mp 90-150° dec.
Tetraphenylborate: [73969-99-0].
$C_{33}H_{47}BP_3Rh$ M 650.3
Yellow powder. Insol. H_2O, THF; mod. sol. MeCN; sol. $MeNO_2$. Mp 120-180° dec.

Jones, R.A. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 511; 1981, 126 (*synth, struct, pmr, P-31 nmr, props*)

$C_9H_{28}Cl_2P_3Rh$ IC-006626

Dichlorohydrotris(trimethylphosphine)rhodium(*III*)

[36350-53-5]



R = Me

M 403.0
Probable *mer*-octahedral struct. with *trans*-Cl. Yellow cryst. Mp 210-219°.

Intille, G.M. *et al, Inorg. Chem.*, 1972, **11**, 695 (*synth, ir*)

$C_9H_{28}P_3Pt^{\oplus}$ IC-006627

Hydrotris(trimethylphosphine)platinum(1+)

Hydridotris(trimethylphosphine)platinum(1+)

$[(Me_3P)_3PtH]^{\oplus}$ (C_{2v})

M 424.3 (ion)
Air-sensitive.
Chloride: [91760-39-3].
$C_9H_{28}ClP_3Pt$ M 459.7
Cryst. (Me_2CO). Mp 158-159°. Ir ν_{Pt-H} 2089 cm^{-1}. Not obt. pure.
Hexafluorophosphate: [115941-42-9].
$C_9H_{28}F_6P_4Pt$ M 569.2
Cream-white solid (CH_2Cl_2/Et_2O).
Tetraphenylborate: [111112-86-8].
$C_{33}H_{48}BP_3Pt$ M 743.5
Cryst. (MeOH). Ir ν_{Pt-H} 2070 cm^{-1}.

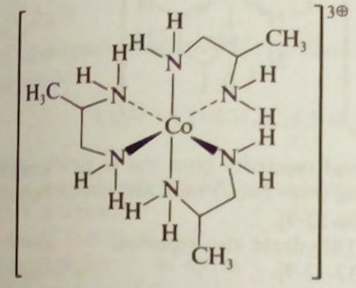
Flood, T.C. *et al, Organometallics*, 1984, **3**, 1795 (*synth, ir, pmr, P-31 nmr*)
Packett, D.L. *et al, Organometallics*, 1988, **7**, 159 (*synth, ir, struct, pmr, P-31 nmr*)
Ramprasad, D. *et al, Inorg. Chem.*, 1988, **27**, 3151 (*synth, pmr, P-31 nmr, props*)

$C_9H_{30}CoN_6^{3\oplus}$ IC-006628

Tris(1,2-propanediamine-*N,N'*)cobalt(*III*)(3+), 9CI

Tris(1,2-diaminopropane)cobalt(III)(3+)

[16786-50-8]



fac-form

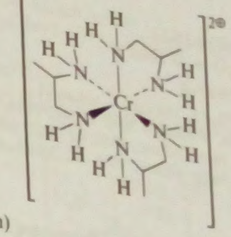
M 281.3 (ion)
Exists as *mer* and *fac*-isomers. Can be resolved. Many derivs. with various counter-ions known.
Trichloride: Golden cryst.
Tribromide: [15627-71-1].
Golden cryst. (dark red). Sl. sol. EtOH, MeOH.
Triiodide: [43223-45-6].
Golden cryst. Sl. sol. MeOH, EtOH.
Hexachloroindate(3−): Orange cryst.
Hexachloromanganate(3−): [20678-75-5].
Brown cryst. $\mu_{eff} = 4.91\ \mu_B$.
Hexachloroferrate(3−): see *Hexachloroferrate*(III)(3−), *IC-017263*
Hexakis(cyano-C)cobaltate(3−): [53730-51-1].
$C_{18}H_{30}Co_2N_{12}$ M 496.3
Orange-red needles. *fac*-form of cation has Co—N 197.1 pm.

[14516-62-2, 15377-75-0, 15412-40-5, 18745-20-5, 20470-19-3, 21019-71-6, 21019-74-9, 22330-27-4, 28816-84-4, 36513-61-8, 41765-65-5, 42566-09-6, 52081-68-2]
Iwasaki, H. *et al, Bull. Chem. Soc. Jpn.*, 1966, **39**, 92 (*cryst struct*)
MacDermott, T.E., *Inorg. Chim. Acta*, 1968, **2**, 81 (*resoln*)
Inorg. Synth., 1968, **11**, 49; 1973, **14**, 57
Kojima, M. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 689 (*resoln, cd*)
Kuroda, R. *et al, Acta Crystallogr., Sect. B*, 1974, **30**, 2126; 1975, **31**, 931 (*cryst struct*)
Danilczuk, E., *Pol. J. Chem.* (*Rocz. Chem.*), 1975, **49**, 467; 1977, **51**, 627 (*thermal dec, synth, uv-vis*)
Gillard, R.D. *et al, Transition Met. Chem.*, 1976, **1**, 223 (*resoln*)
Mason, S.F. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 937 (*cd*)
Bell, C.F. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 773 (*ir*)
Scoville, A.N. *et al, Inorg. Chem.*, 1983, **22**, 3514 (*md, mössbauer, magnetism*)
Tsuchuya, R. *et al, Thermochim. Acta*, 1985, **88**, 289 (*stability*)

$C_9H_{30}CrN_6^{2\oplus}$ IC-006629

Tris(1,2-propanediamine)chromium(*II*)(2+), 8CI

Tris(propylenediamine)chromium(II)(2+)

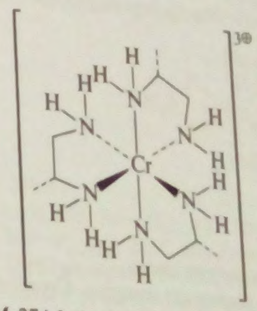


M 274.3 (ion)
Octahedral cation. Salts all high spin.
Dichloride: [33850-17-8].
$C_9H_{30}Cl_2CrN_6$ M 345.2
Air-sensitive light blue solid.
Dibromide: [33850-18-9].
Air-sensitive blue solid.
Diiodide: [33850-19-0].
Air-sensitive blue solid.
Larkworthy, L.F. *et al, J. Chem. Soc. A*, 1971, 2766 (*synth, props*)

$C_9H_{30}CrN_6^{3\oplus}$ IC-006630

Tris(1,2-propanediamine-*N,N'*)chromium(*III*)(3+), 11CI, 10CI, 9CI

[41507-05-5]



Δ(*R*)(*R*)(*R*)-*form*

M 274.3 (ion)
fac-Octahedral cation. Chiral ligands give rise to diastereomers which can be separated chromatographically.
Trichloride: [14949-95-2].
Yellow solid + H_2O. Dehydrates at 70-100° and loses some amine becoming *cis*- then *trans*-$[CrCl_2(diamine)_2]$ Cl.
Tribromide: [17631-70-8].
Yellow solid + H_2O. Loses H_2O at 50-90° and some amine at 180-220°.
Trithiocyanate: [22754-50-3].

Yellow solid. Loses amine at 120-150°; turns orange and dec.

Δ-(R)(R)(R)-form [51002-44-9]
(−)-form
Trichloride: [96412-04-3].
Yellow solid + $1.5H_2O$.

Δ-(S)(S)(S)-form
(−)-form
Trichloride: [96479-36-6].
Solid + $3H_2O$.

Δ-(R)(R)(S)-form
(−)-form
Trichloride: [96479-34-4].
Solid + $0.5H_2O$ + 0.75NaCl.

Δ-(R)(S)(S)-form
(−)-form
Trichloride: [96479-35-5].
Solid + $2H_2O$ + 0.5NaCl.

[15053-78-8, 28816-83-3]

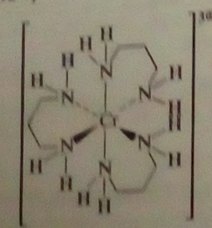
Inorg. Synth., 1972, **13**, 184 (*synth, chloride*)
Gillard, R.D. *et al, Transition Met. Chem.*, 1976, **1**, 223 (*resoln*)
Uehara, A. *et al, Inorg. Chem.*, 1982, **21**, 2422 (*thermal dec*)
Kaizaki, S. *et al, Inorg. Chem.*, 1985, **24**, 2080 (*cd, uv-vis, Δ-form*)

$C_9H_{30}CrN_6^{3\oplus}$ IC-006631

Tris(1,3-propanediamine-*N,N'*)chromium(*III*)(3+), 1ICl, 1OCl, 9Cl

Tris(trimethylenediamine)chromium(3+)

[15276-12-7]



Δ-form

M 274.3 (ion)

Δ-form [78420-64-1]
(+)-form
Triperchlorate: [29753-87-5].

Λ-form
(−)-form
Tribromide: [39000-79-8].
Microcryst. + H_2O.

(±)-form
Trichloride: [17978-78-8].
Synth. from 1,3-propanediamine and a chlorodimethylsulfoxide chromium complex. Cryst. + H_2O (aq. HCl).

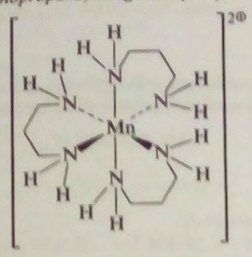
Pentakis(cyano-C)nickelate(3−): see *Pentakis(cyano-C)nickelate*(II)(3−), *IC-004836*

Pedersen, E., *Acta Chem. Scand.*, 1970, **24**, 3362 (*synth*)
Rancke-Madsen, M. *et al, Acta Chem. Scand.*, 1972, **26**, 3405 (*cd, resoln*)
Jensen, H.P., *Acta Chem. Scand., Ser. A*, 1981, **35**, 127 (*cd, theory*)

$C_9H_{30}MnN_6^{2\oplus}$ IC-006632

Tris(1,3-propanediamine-*N,N'*)manganese(*II*)(2+), 9Cl

Tris(1,3-diaminopropane)manganese(2+)



M 277.3 (ion)
Approx. octahedral.

Diperchlorate: [52632-84-5].
Synth. from $MnCl_2$ + $NaClO_4$ in EtOH followed by removal of NaCl and addition of $H_2N(CH_2)_3NH_2$. White solid.

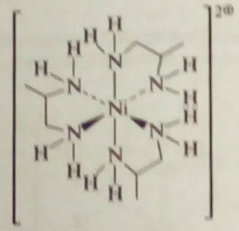
Chiswell, B. *et al, Inorg. Chim. Acta*, 1973, **7**, 707 (*synth, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, D3, 43 (*rev, bibl*)

$C_9H_{30}N_6Ni^{2\oplus}$ IC-006633

Tris(1,2-propanediamine)nickel(*II*)(2+)

Tris(1,2-diaminopropane)nickel(II)(2+), *8Cl. Tris(1,2-propylenediamine)nickel*(II)(2+)

[20142-36-3]



M 281.0 (ion)
Octahedral. Ligand reactivity gives rise to new complexes. Easily prepared from Ni(*II*) salts and excess ligand.

Dichloride: [39494-22-9].
Mauve solid. Dihydrate also reported.
Dibromide: [15337-12-9].
Mauve solid + $1H_2O$.
Diphenyldithiophosphinate: [53837-29-9].
Pink cryst.

[15282-51-6]

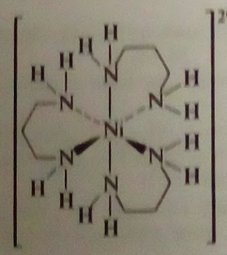
Werner, A. *et al, Z. Anorg. Allg. Chem.*, 1899, **21**, 210.
Inorg. Synth., 1960, **6**, 200.
Mukherjee, R.N. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 1418.

$C_9H_{30}N_6Ni^{2\oplus}$ IC-006634

Tris(1,3-propanediamine-*N,N'*)nickel(2+), 9Cl

Tris(1,3-diaminopropane)nickel(II).

[18347-71-2]



M 281.0 (ion)

Many salts known, less stable than ethylenediamine analogues.

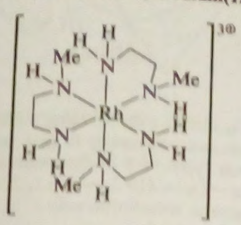
Dichloride: [88119-38-4].
Blue-violet solid + $2H_2O$. Anhydrous formulation also reported, but possibly same material.
Nitrate: [41782-15-4].
Perchlorate: [94387-32-3].
Mauve cryst.
▷ Potentially explosive.

[20577-76-8]

House, D.A. *et al, J. Am. Chem. Soc.*, 1964, **86**, 223 (*synth, uv-vis*)
Vezzosi, I.M. *et al, Inorg. Chim. Acta*, 1985, **97**, 195 (*synth, cryst struct*)

$C_9H_{30}N_6Rh^{3\oplus}$ IC-006635

Tris(*N*-methylethylenediamine)rhodium(*III*)(3+)



M 325.2 (ion)
Octahedral, detailed config. not investigated.

Trisiodide: Synth. by addn. of large excess of amine to $RhCl_3.3H_2O$ followed by metathesis with KI. White cryst. (H_2O). λ_{max} 312 (ε 300).

Watt, G.W. *et al, J. Am. Chem. Soc.*, 1967, **89**, 1814 (*synth, ir, uv*)

$C_9H_{30}N_6Rh^{3\oplus}$ IC-006636

Tris(1,2-propanediamine-*N,N'*)rhodium(3+)

[41507-06-6]

$Rh[H_2NCH(CH_3)CH_2NH_2]_3^{3\oplus}$

M 325.2 (ion)
Various optically-active forms are known. Prepd. from $Rh^{3\oplus}$ + ligand.

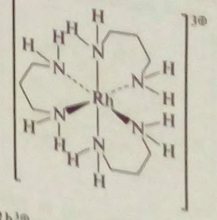
Trichloride: [14175-72-5].
$C_9H_{30}Cl_3N_6Rh$ M 431.6
White cryst. + H_2O.

[27661-97-8, 63527-68-4]

Schmidtke, H.-H., *Z. Physik. Chem.*, 1963, **38**, 170 (*synth, uv*)
Gillard, R.D. *et al, J. Chem. Soc.*, 1965, 1951 (*synth*)
Andersen, P. *et al, Acta Chem. Scand.*, 1969, **23**, 3027 (*abs config*)
Schreiber, S. *et al, Inorg. Chem.*, 1977, **16**, 3190 (*N-15 nmr*)
Hearnon, J.A. *et al, Inorg. Chim. Acta*, 1977, **23**, 95 (*synth, abs config*)
Gillard, R.D., *Inorg. Chim. Acta*, 1977, **25**, L93 (*abs config*)

$C_9H_{30}N_6Rh^{3\oplus}$ IC-006637

Tris(1,3-propanediamine-*N,N'*)rhodium(3+)



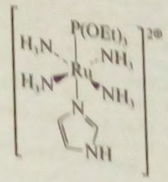
M 325.2 (ion)
Prepd. from $Rh^{3\oplus}$ + ligand. No phys. props. reported.

[64175-36-6]

Inorg. Synth., 1970, **12**, 269 (*synth*)
Schreiber, S. *et al, Inorg. Chem.*, 1977, **16**, 3190 (*N-15 nmr*)

$C_9H_{31}N_6O_3PRu^{2\oplus}$ IC-006638

Tetraammine(1*H*-imidazole-*N*³)(triethyl phosphite-*P*)ruthenium(*II*)(2+), 9Cl



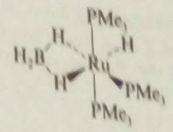
M 403.4 (ion)
Prepd. by treating Tetraammineaqua(triethyl phosphite-*P*)ruthenium(*II*)(2+), IC-005552 with an excess of imidazole. Sol. H_2O.

Bis-hexafluorophosphate: [64939-08-8].
White cryst.

Franco, D.W. *et al, Inorg. Chem.*, 1978, **17**, 571 (*synth, uv*)

$C_9H_{32}BP_3Ru$ IC-006639

Hydro[tetrahydroborato(1−)-*H,H'*]tris(trimethylphosphine)ruthenium(*II*)



M 345.1
Ru—H 149, Ru—H_{eq} 183, Ru—$P_{trans\,H}$ 230.5, Ru—$P_{trans\,eq}$ 225.9 pm. Prepd. by treating Dichlorotetrakis(trimethylphosphine)ruthenium(*II*), IC-008227 or dichloride of Di-μ-chlorooctakis(trimethylphosphine)diruthenium(*II*)(2+), IC-011702 with excess $LiBH_4$. Extremely air-sensitive yellow cryst. Sol. C_6H_6. Mp 116-119°. Ir ν_{eq} 2383, 2369, 2318 (nujol); $\nu_{eq\,H}$ 1932 cm^{-1}.

Statler, J.A. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1731 (*synth, ir, pmr, P-31 nmr, cryst struct*)

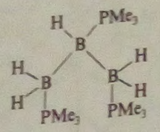
IC-006640

$C_9H_{32}B_3P_3$

Tris(trimethylphosphine)triborane(5)

Triborane(5) compd. with trimethylphosphine (1:3), 10CI

[73636-27-8]



M 265.7

hypho-. Not isol.

Kameda, M. *et al, Inorg. Chem.*, 1980, **19**, 2288 (*synth, B-11 nmr*)

IC-006641

$C_9H_{32}P_3W^{\ominus}$

Pentahydrotris(trimethylphosphine)tungstate(*IV*)(1−), 11CI

$[WH_5(PMe_3)_3]^{\ominus}$

M 417.1 (ion)

(15-Crown-5)Na salt: [101461-89-6].
Synth. from $W(PMe_3)_3H_6$ in THF with NaH then 15-crown-5 added. Yellow cryst. (THF). W—Na 321 pm.

(18-Crown-6)K salt: [101461-90-9].
Synth. from $W(PMe_3)_3H_6$ in THF with KH then 18-crown-6 added. Yellow cryst. (THF). W—K 366 pm.

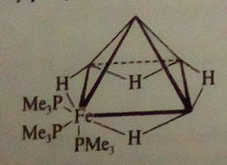
Bandy, J.A. *et al, J. Chem. Soc., Chem. Commun.*, 1985, 1462 (*cryst struct, pmr, P-31 nmr*)

Barron, A.R. *et al, J. Chem. Soc., Chem. Commun.*, 1986, 81 (*synth, cryst struct*)

IC-006642

$C_9H_{35}B_4FeP_3$

2-[Tris(trimethylphosphine)ferra]pentaborane(9)



M 335.3

nido-. Air-stable orange cryst. Sol. C_6H_6.

Grebenik, P.D. *et al, J. Chem. Soc., Chem. Commun.*, 1990, 1234 (*synth, pmr, B-11 nmr, P-31 nmr, cryst struct*)

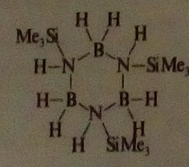
IC-006643

$C_9H_{36}B_3N_3Si_3$

Hexahydro-1,3,5-tris(trimethylsilyl)borazine, 11CI

1,3,5-Tris(trimethylsilyl)cyclotriborazane

[81132-97-0]



M 303.0

White solid which slowly cryst. from a clear colourless liq. (low-boiling distillate from reaction mixt.). Mp 117° dec.

Nutt, W.R. *et al, Inorg. Chem.*, 1982, **21**, 2469 (*synth, props, pmr, B-11 nmr*)

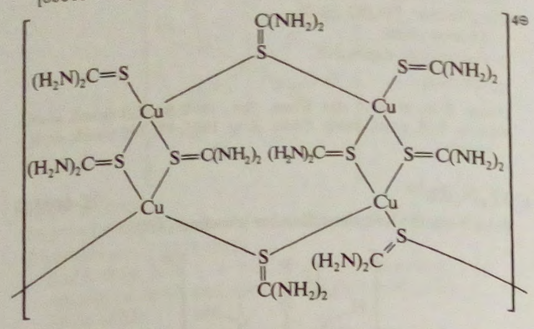
IC-006644

$C_9H_{36}Cu_4N_{18}S_9^{4\ominus}$

Nonakis(thiourea)tetracopper(*I*)(4+)

Hexakis[μ-(thiourea-S:S)]tris(thiourea-S)tetracopper(4+), 11CI

[60618-39-5]



M 939.2 (ion)

Rectangle of Cu atoms with bridging sulfurs from thiourea groups, which can polymerise to give infinite lattice. Three different types of S bridge exist. Interatomic distances: Cu—Cu ~419.2, ~416.1, 270.7 pm. Model for canine hepatic metallothionein.

Tetranitrate: Cryst. (H_2O).

Vranka, R.G. *et al, J. Am. Chem. Soc.*, 1966, **88**, 4270 (*synth, cryst struct*)

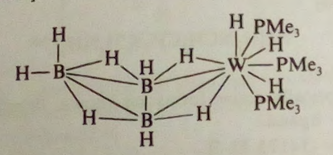
Freedman, J.H. *et al, Biochemistry*, 1986, **25**, 2342 (*exafs, model studies*)

IC-006645

$C_9H_{38}B_3P_3W$

Trihydro[(1,2-η)-octahydrotriborato(1−)-H^1,H^2]tris(trimethylphosphine)tungsten, 12CI

[120730-18-9]



M 455.6

arachno-. Yellow-brown cryst. (pet. ether). Sol. pet. ether.

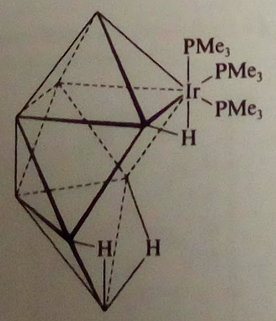
Grebenik, P.D. *et al, J. Organomet. Chem.*, 1988, **345**, C31 (*synth, pmr, B-11 nmr, P-31 nmr*)

IC-006646

$C_9H_{38}B_8IrP_3$

Tris(trimethylphosphine)[(3,4,5,6-η)undecahydrooctaborato(3−)-H^6]iridium, 11CI

[96029-11-7]



M 518.0

nido-. Sol. toluene.

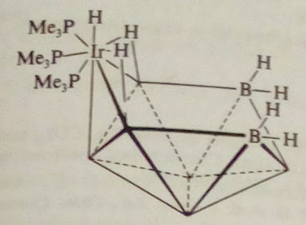
Bould, J. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 2477 (*synth, B-11 nmr*)

IC-006647

$C_9H_{40}B_8IrP_3$

[η³-Dodecahydrooctaborato(2−)]hydrotris(trimethylphosphine)iridium, 11CI

[95013-17-5]



M 520.0

arachno-. Colourless cryst. Sol. CH_2Cl_2.

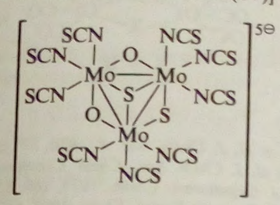
Greenwood, N.N. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1903 (*synth, B-11 nmr, pmr, P-31 nmr*)

IC-006648

$C_9Mo_3N_9O_2S_{11}^{5\ominus}$

Di-μ-oxononakis(thiocyanato-*N*)-μ-thioxo-μ_3-thioxotrimolybdate(*IV*)(5−), 11CI

Bis(μ_2-oxo)-μ_2-sulfido-μ_3-sulfidotris[triisothiocyanatomolybdenum(IV)]



M 906.7 (ion)

Incomplete cubane-type core struct. Interatomic distances: Mo—Mo 271.5, 263.5. 263.5 pm.

Penta-pyridinium salt: [103138-80-3].
Greenish-brown cryst. + $2H_2O$.

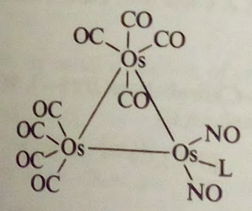
Shibahara, T. *et al, Inorg. Chim. Acta*, 1986, **113**, L19 (*cryst struct, synth, uv-vis*)

IC-006649

$C_9N_2O_{11}Os_3$

Nonacarbonyldinitrosyltriosmium, 10CI

[64973-41-7]



L = CO

M 882.7

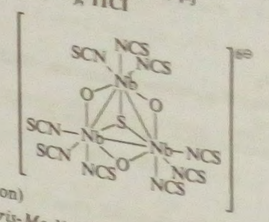
Dark-red cryst. (pentane).

Bhaduri, S. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 557 (*synth, ir, props, cmr, ms*)

IC-006650

$C_9N_9Nb_3O_9S_{10}^{6\ominus}$

Tri-μ-oxononakis(thiocyanato-*N*)-μ_3-thioxotriniobate(6−), 11CI



M 881.5 (ion)

Tri-NH_4, tris-Me_4N salt: [106333-00-0].
Synth. by adding aq. HCl to a THF soln. of Nb_2Cl_6(tetrahydrothiophene)$_3$ and eluting the product from an ion-exchange column with $SCN^{\ominus}$. Black solid + 1MeOH (MeOH).

Cotton, F.A. *et al, J. Chem. Soc., Chem. Commun.*, 1986, 1276 (*synth, cryst struct*)

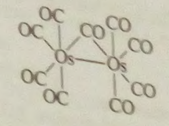
IC-006651

$C_9O_9Os_2$

μ-Carbonyloctacarbonyldiosmium, 8CI

Nonacarbonyldiosmium. Diosmium nonacarbonyl. Diosmium enneacarbonyl

[28411-13-4]



M 632.4

Thermally-sensitive and photosensitive orange-yellow cryst. Sol. hydrocarbons, unlike $Fe_2(CO)_9$. Mp 64-67° dec.

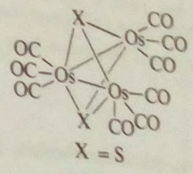
Moss, J.R. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 95 (*synth, ir, ms*)

IC-006652

$C_9O_9Os_3S_2$

Nonacarbonyldi-μ_3-thioxotriosmium, 10CI

[72282-40-7]



X = S

M 886.8

Yellow cryst. (hexane).

Johnson, B.F.G. *et al, J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir*)

Adams, R.D. *et al, J. Am. Chem. Soc.*, 1982, **104**, 4115 (*synth*)

Adams, R.D. *et al, Organometallics*, 1983, **2**, 144 (*struct*)

IC-006653

$C_9O_9Os_3Se_2$

Nonacarbonyldi-μ_3-selenoxotriosmium, 10CI

[72282-41-8]

As Nonacarbonyldi-μ_3-thioxotriosmium, IC-006652 with

X = Se

M 980.6

Johnson, B.F.G. *et al. J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir*)
Johnson, B.F.G. *et al. Acta Crystallogr., Sect. B*, 1981, **37**, 1731 (*struct*)

IC-006654

$C_9O_9Os_3Te_2$
Nonacarbonyldi-μ_3-telluroxotriosmium, 10Cl
[72282-42-9]
As Nonacarbonyldi-μ_3-thioxotriosmium, IC-006652 with

X = Te

M 1077.8
Johnson, B.F.G. *et al. J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir*)

IC-006655

$C_9O_9Re_2^{2\ominus}$
μ-Carboyloctacarbonyldirhenate(2−), 10Cl
Nonacarbonyldirhenate(2−)

$[Re_2(CO)_9]^{2\ominus}$

M 624.5 (ion)
Di-K salt: [86940-26-9].
Synth. from K[CH(OR)$_2$CH$_2$CH$_2$]BH and $Re_2(CO)_{10}$.
Orange powder (THF/hexane). Dec. at 120-140°. Ir 2059w, 2010m, 1966s, 1924s, 1880m, 1860m cm^{-1} (THF).
Gladysz, J.A. *et al. J. Am. Chem. Soc.*, 1978, **100**, 2545 (*synth, ir*)
Tam, W. *et al. Inorg. Chem.*, 1983, **22**, 1413 (*synth*)

IC-006656

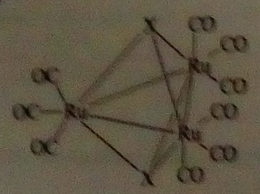
$C_9O_9Ru_3$
Nonacarbonyldiruthenium
μ-Carbonyloctacarbonyldiruthenium, 6Cl. Ruthenium carbonyl ($Ru_3(CO)_{12}$). Diruthenium enneacarbonyl. Diruthenium nonacarbonyl
[63128-11-4]

$Ru_2(CO)_9$

M 494.2
Struct. not detd. V. early reports of $Ru_2(CO)_9$ as an orange solid are in error– it was in fact $Ru_3(CO)_{12}$.
Synth. by low temp. (-40°) irradiation of $Ru_3(CO)_{12}$ in heptane. Not isol. pure; v. unstable at r.t. Sol. heptane. Ir ν_{CO} 2077, 2035, 1814 cm^{-1} (heptane).
Moss, J.R. *et al. J. Chem. Soc., Dalton Trans.*, 1977, 95 (*synth, ir, rea*)

IC-006657

$C_9O_9Ru_3S_3$
Nonacarbonyldi-μ_3-thioxotriruthenium, 10Cl
Nonacarbonyldisulfidotriruthenium
[72282-38-3]



X = S

M 619.4
Synth. by the reaction between $Ru_3(CO)_{12}$ and elemental sulfur under CO/H_2 (35 atm). Characterised spectroscopically. Ir ν_{CO} 2078, 2057, 2024, 2016 cm^{-1}.
Johnson, B.F.G. *et al. J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir*)

IC-006658

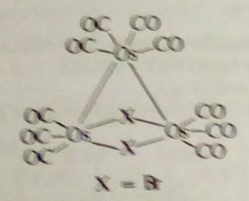
$C_9O_9Ru_3Se_2$
Nonacarbonyldi-μ_3-selenoxotriruthenium, 10Cl
Nonacarbonyldiselenidotriruthenium
[72282-39-4]
As Nonacarbonyldi-μ_3-thioxotriruthenium, IC-006657 with

X = Se

M 713.2
Synth. by the reaction between $Ru_3(CO)_{12}$ and Se under CO/H_2 (35 atm). Characterised spectroscopically. Ir ν_{CO} 2076, 2053, 2019, 2010 cm^{-1}.
Johnson, B.F.G. *et al. J. Chem. Soc., Chem. Commun.*, 1979, 719 (*synth, ir*)

IC-006659

$C_{10}Br_2O_{10}Os_3$
Di-μ-bromodecacarbonyltriosmium, 8Cl
[28109-19-5]



X = Br

M 1010.5
Yellow crystl.
Deeming, A.J. *et al. J. Chem. Soc. A*, 1970, 897 (*synth, ir*)
Bryan, E.G. *et al. J. Chem. Soc., Chem. Commun.*, 1977, 329 (*cmr*)
Viglio, G.A., *J. Organomet. Chem.*, 1979, **169**, 83 (*ms*)
Aleksandrov, G.G. *et al. Koord. Khim.*, 1980, **6**, 626 (*struct*)

IC-006660

$C_{10}Cl_2O_{10}Os_3$
Decacarbonyldi-μ-chlorotriosmium, 10Cl
[64387-08-2]
As Di-μ-bromodecacarbonyltriosmium, IC-006659 with

X = Cl

M 921.6
Yellow plates. Subl.$_{0.15}$ 80°.
Deeming, A.J. *et al. J. Chem. Soc. A*, 1970, 897 (*synth, ir*)
Bryan, E.G. *et al. J. Chem. Soc., Chem. Commun.*, 1977, 329 (*cmr*)

IC-006661

$C_{10}Co_2N_{10}^{6\ominus}$
Decakis(cyano-*C*)dicobaltate(*II*)(6−), 9Cl
Decacyanodicobaltate(II)

$[(NC)_5Co{-}Co(CN)_5]^{6\ominus}$

M 378.0 (ion)
Isoelectronic and isosteric with $Mn_2(CO)_{10}$.
Hexa-Na salt: Red-violet solid.
Hexa-K salt: Blue-violet solid.
Tri-Ba salt: [38856-44-9].
Violet needles + $13H_2O$.
Nast, R. *et al. Z. Anorg. Allg. Chem.*, 1961, **312**, 314 (*synth, ir*)

Griffith, W.P. *et al. J. Chem. Soc. A*, 1969, 834 (*ir, raman*)
Simon, G.L. *et al. J. Am. Chem. Soc.*, 1972, **94**, 7654 (*synth, cryst struct*)

IC-006662

$C_{10}Co_2N_{10}O_2^{8\ominus}$
Decakis(cyano-*C*)(μ-(peroxy-*O:O'*))dicobaltate(*II*)(8−), 9Cl
μ-Peroxobis[pentacyanocobaltate(II)]

$[(NC)_5Co{-}O{-}O{-}Co(CN)_5]^{8\ominus}$

M 410.0 (ion)
Octa-K salt, bis-KNO_3 double salt: [53513-76-1].
Orange cryst. + $4H_2O$.
Fronzek, F.R. *et al. Inorg. Chim. Acta*, 1974, **9**, 143 (*synth, cryst struct*)

IC-006663

$C_{10}Co_2N_{10}O_2^{6\ominus}$
Decakis(cyano-*C*)(μ-(peroxy-*O:O'*))dicobaltate(*III*)(6−), 10Cl
Decacyanoperoxodicobaltate(III)
[25488-84-4]

$[(NC)_5Co{-}O{-}O{-}Co(CN)_5]^{6\ominus}$

M 410.0 (ion)
Hexa-K salt: [23733-07-5].
Brown solid.
Shin, A. *et al. J. Am. Chem. Soc.*, 1961, **83**, 509 (*synth, ir*)
Shibata, T. *et al. Bull. Chem. Soc. Jpn.*, 1970, **51**, 1374 (*raman, ir*)

IC-006664

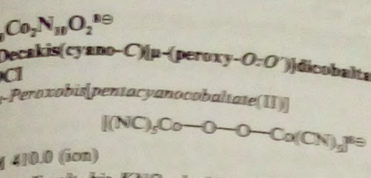
$C_{10}Co_2N_{10}O_2^{8\ominus}$
Decakis(cyano-*C*)-μ-hyperoxodicobaltate(*III*)(5−)
μ-Superoxobis[pentacyanocobaltate(III)]

$[(NC)_5Co(O_2)Co(CN)_5]^{5\ominus}$

M 410.0 (ion)
Penta-K salt: [12557-90-3].
Red solid. Sol. H_2O.
Inorg. Synth., 1970, **12**, 202 (*synth*)

IC-006665

$C_{10}Co_2N_{10}O_2S_2^{4\ominus}$
[Decakis(cyano-*C*)μ-[monothiosulfito(2−)-*S:S'*]]dicobaltate(*III*)(6−), 11Cl



M 474.1 (ion)
Octahedral. Obt. by aerial oxidation of corresp. disulfido complex.
Hexa-K salt: [81611-01-0].
Orange cryst. + H_2O + EtOH.
Fronzek, F.R. *et al. J. Am. Chem. Soc.*, 1982, **104**, 3382 (*synth, w. cryst struct*)

IC-006666

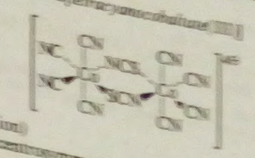
$C_{10}Co_2N_{10}S_2^{4\ominus}$
Decakis(cyano-*C*)μ-(dithio-*S:S'*)]dicobaltate(6−), 9Cl
μ-Disulfidobis[pentacyanocobaltate(III)](6−)

$[(NC)_5CoSSCo(CN)_5]^{6\ominus}$

M 442.1 (ion)
Hexa-K salt: [42075-66-1].
Brown cryst. Spar. sol. H_2O.
Siebert, H. *et al. Z. Anorg. Allg. Chem.*, 1973, **399**, 107 (*synth, ir, raman, str*)

IC-006667

$C_{10}Co_2N_{10}S_2^{4\ominus}$
Bis[μ-(thiocyanato-*N:S*)]tetrakis(cyano-*C*)dicobaltate(*III*)(4−)
Di-μ-(thiocyanato)bis[pentacyanocobaltate(III)]



M 442.1 (ion)
Probably centrosymmetric as shown.
Tetra-K salt: Brown solid.
Burmeister, J.L. *et al. Inorg. Chem.*, 1965, **4**, 902 (*synth, ir*)

IC-006668

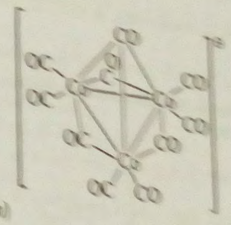
$C_{10}Co_2N_{10}Se_2^{4\ominus}$
Decakis(cyano-*C*)[μ-(diseleno-*Se:Se'*)]dicobaltate(*II*)(6−), 9Cl
μ-Diselenatobis[pentacyanocobaltate(III)](6−)

$[(NC)_5Co(Se)_2Co(CN)_5]^{6\ominus}$

M 555.9 (ion)
Binuclear anion.
Hexa-K salt: [42740-42-1].
Black cryst. + $5H_2O$. Sol. H_2O.
Siebert, H. *et al. Z. Anorg. Allg. Chem.*, 1973, **399**, 107 (*synth, ir, raman, str*)

IC-006669

$C_{10}Co_2O_{10}^{\ominus}$
Tris-μ-carbonyl-μ$_3$-carbonyl-heptacarbonyltriiodate(1−), 10Cl
Decacarbonyltriiodate(1−)
[12557-48-4]



M 456.9 (ion)
Li salt:
$C_{10}Co_2LiO_{10}$ M 463.8
Black cryst. (Et_2O) forming red soln. Ir ν_{CO} 2080-2000, 1850, 1600 cm^{-1} (THF).
Fieldhouse, S.A. *et al. J. Chem. Soc., Chem. Commun.*, 1970, 181 (*synth, ir*)

IC-006670

$C_{10}Cr_2IO_{10}^{\ominus}$
Decacarbonyl-μ-iodidochromate(1−), 8Cl

$[(OC)_5Cr{-}I{-}Cr(CO)_5]^{\ominus}$

M 459.0 (ion)
Bis(triphenylphosphine)iminium salt: [21637-80-9].

Red cryst. Mp 109-110°.

Ruff, J.K., *Inorg. Chem.*, 1968, **7**, 1821 (*synth*)
Dahl, L.F. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 7327 (*cryst struct*)

IC-006671

$C_{10}CrO_{10}Re^{\ominus}$

Pentacarbonyl(pentacarbonylrhenate)chromate(1 –), 9CI

Decacarbonylchromaterhenate(1 –)

$$[(OC)_5Re—Cr(CO)_5]^{\ominus}$$

M 518.3 (ion)
[15376-98-4].
Orange cryst. (EtOH aq.). Ir ν_{CO} 2078w, 1985s, 1961vs, 1928m, 1888s, 1858m cm^{-1} (THF).

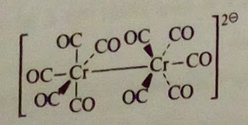
Anders, U. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 539 (*synth, ir*)
Johnson, J.R. *et al*, *Inorg. Chem.*, 1975, **14**, 1053 (*ir, uv, raman*)

IC-006672

$C_{10}Cr_2O_{10}^{2\ominus}$

Decacarbonyldichromate(2 –), 9CI

[45264-01-5]



M 384.0 (ion)
Di-Na salt: [15616-67-8].
$C_{10}Cr_2Na_2O_{10}$ M 430.0
Yellow cryst.
Di-K salt: [57348-61-5].
Yellow cryst.
Bis-Et_4N salt: [15682-68-5].
Yellow cryst.
Bis[bis(triphenylphosphine)iminium] salt: [49736-18-7].
Dark-yellow cryst. Sol. CH_2Cl_2. Mp 185-189° dec.

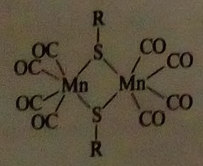
Hayter, R.E., *J. Am. Chem. Soc.*, 1966, **88**, 4376 (*props*)
Ruff, J.K., *Inorg. Chem.*, 1967, **6**, 2080 (*props*)
Dahl, L.F. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 7312 (*cryst struct*)
Ruff, J.K. *et al*, *J. Organomet. Chem.*, 1971, **33**, C64 (*props*)
Inorg. Synth., 1974, **15**, 89 (*synth*)
Unguvenasu, C. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 388 (*synth*)
Behrens, H. *et al*, *Z. Naturforsch., B*, 1977, **32**, 1105 (*props*)

IC-006673

$C_{10}F_6Mn_2O_8S_2$

Octacarbonylbis[μ-(trifluoromethanethiolato)] dimanganese, 9CI

[21239-57-6]



R = CF_3

M 536.1
Synth. from $MnBr(CO)_5$ and CF_3SAg in CH_2Cl_2. Orange or yellow cryst. (CH_2Cl_2/hexane). Mp 99°. $Subl._{0.01}$ 70°. Ir ν_{CO} 2098s, 2091w, 2038vs, 2026s, 1996vs, 1967w cm^{-1}.
▷ OP1325000.

King, R.B. *et al*, *Inorg. Chem.*, 1968, **8**, 2540 (*synth, F-19 nmr, ir*)
Grobe, J. *et al*, *Z. Anorg. Allg. Chem.*, 1969, **371**, 123 (*synth, ir, F-19 nmr*)
Chaudhuri, M.K. *et al*, *Org. Mass Spectrom.*, 1981, **16**, 534 (*ms*)

IC-006674

$C_{10}F_6Mn_2O_8Se_2$

Octacarbonylbis[μ-(trifluoromethaneselenolato)] dimanganese, 9CI

Bis(trifluoromethaneselenolato)octacarbonyldimanganese

[15651-21-5]

As Octacarbonyldi-μ-selenyldimanganese, IC-005890 with

R = CF_3

M 629.8
Synth. from $HMn(CO)_5$ and $CF_3SeSeCF_3$. Orange-brown cryst. (CH_2Cl_2/hexane). Mp 96-97°. $Subl._{0.001}$ 50°. Ir ν_{CO} 2100vs, 2060vs, 2020vs, 1955vs cm^{-1} (KBr).

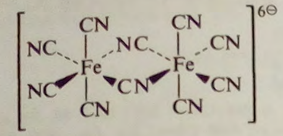
Welcman, N. *et al*, *J. Chem. Soc.*, 1965, 7515 (*synth, ir*)
Grobe, J. *et al*, *Z. Anorg. Allg. Chem.*, 1969, **371**, 123 (*synth, ir, F-19 nmr*)
Marsden, C.J. *et al*, *J. Organomet. Chem.*, 1972, **40**, 175 (*struct*)
Chaudhuri, M.K. *et al*, *Org. Mass Spectrom.*, 1981, **16**, 534 (*ms*)

IC-006675

$C_{10}Fe_2N_{10}^{6\ominus}$

Bis[μ-(cyano-*C*:*N*)]octakis(cyano-*C*)diferrate(6 –), 11CI

Di-μ-cyanobis[tetracyanoferrate(II)](6 –).
Decacyanodiferrate



M 371.8 (ion)
In equil. with mononuclear ions in aq. soln., dimer favoured at high conc., at low temp., or on addn. of EtOH. Obt. by dimerisation of $[Fe(CN)_5(OH_2)]^{3\ominus}$. Oxidises to give first, green $[Fe_2(CN)_{10}]^{5\ominus}$ and then purple $[Fe_2(CN)_{10}]^{4\ominus}$.
Hexa-Na salt: [28777-10-8].
Oxidised by Br_2 to $Na_4[Fe(CN)_{10}]$, occurring as octahydrate.
Tri-Pb(II) salt:
$C_{10}Fe_2N_{10}Pb_3$ M 993.4

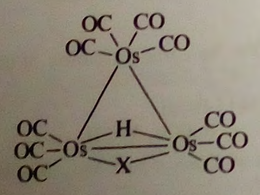
Emschwiller, G. *et al*, *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1967, **265**, 281; 1970, **270**, 1362; 1972, **274**, 1500 (*synth, photol, therm props, dissoc*)
Emschwiller, G. *et al*, *Chem. Phys. Lett.*, 1970, **5**, 561 (*uv*)
Wolfe, S.K. *et al*, *Inorg. Chem.*, 1974, **13**, 2567 (*soln kinetics*)
Davies, G. *et al*, *Inorg. Chim. Acta*, 1976, **19**, L3 (*equil*)
James, A.D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1182 (*kinetics*)

IC-006676

$C_{10}HBrO_{10}Os_3$

μ-Bromodecacarbonyl-μ-hydrotriosmium

[61199-98-2]



X = Br

M 931.6
Yellow cryst. (hexane).

Bryan, E.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1328; 1978, 196 (*synth, cmr*)
Churchill, M.R. *et al*, *Inorg. Chem.*, 1979, **18**, 3261 (*struct*)

$C_{10}HClO_{10}Os_3$

Decacarbonyl-μ-chloro-μ-hydrotriosmium, 10CI

IC-006677

[12557-93-6]

As μ-Bromodecacarbonyl-μ-hydrotriosmium, IC-006676 with

X = Cl

M 887.1
Yellow cryst. (hexane).

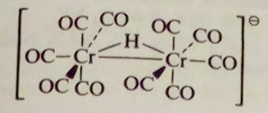
Bryan, E.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1328; 1978, 196 (*synth, cmr*)
Churchill, M.R. *et al*, *Inorg. Chem.*, 1979, **18**, 1926 (*struct*)

$C_{10}HCr_2O_{10}^{\ominus}$

Decacarbonyl-μ-hydrodichromate(1 –), 10CI

IC-006678

[73740-63-3]



M 385.1 (ion)
Et_4N salt: [16924-36-0].
Yellow cryst., v. air-sensitive.
Bis(triphenylphosphine)iminium salt: [62341-83-7].
Yellow cryst.

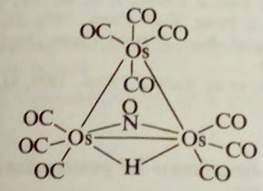
Hayter, R.J., *J. Am. Chem. Soc.*, 1966, **88**, 4376 (*synth*)
Dahl, L.F. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 7312 (*cryst struct*)
Dahl, L.F. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 4497.
Cooper, C.B. *et al*, *Adv. Chem. Ser.*, 1978, **167**, 232 (*ir, raman*)

$C_{10}HNO_{11}Os_3$

Decacarbonyl-μ-hydro-μ-nitrosyltriosmium, 10CI

IC-006679

[73238-03-6]



M 881.7
Characterised spectroscopically.

Johnson, B.F.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 99 (*synth, ir*)
Stevens, R.E. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 4981 (*synth*)

$C_{10}HO_{10}W_2^{\ominus}$

Decacarbonyl-μ-hydroditungstate(1 –)

IC-006680

[19773-10-5]

$$[(OC)_5W—H—W(CO)_5]^{\ominus}$$

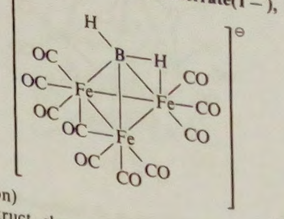
M 648.8 (ion)
$Et_4N^{\oplus}$ salt adopts linear eclipsed struct. $PPN^{\oplus}$ salt adopts bent staggered struct.
Et_4N salt: [12083-01-1].
Yellow cryst.
Bis(triphenylphosphine)iminium salt: [56172-01-1].
Yellow prisms (CH_2Cl_2/Et_2O).
Ph_4P salt: [97012-34-5].
Light-yellow cryst. (EtOH/toluene).

Hayter, R.G., *J. Am. Chem. Soc.*, 1966, **88**, 4376 (*synth*)
Gray, H.B. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 3073 (*synth, ir*)
Wilson, R.D. *et al*, *J. Organomet. Chem.*, 1975, **91**, C49 (*cryst struct*)
Bau, R. *et al*, *Acc. Chem. Res.*, 1979, **12**, 176 (*cryst struct*)
Hart, D.W. *et al*, *Organometallics*, 1985, **4**, 1590 (*struct*)

$C_{10}H_2BFe_3O_{10}^{\ominus}$

μ-Boryl-μ-carbonylnonacarbonyltriferrate(1 –), 11CI

IC-006681



M 460.4 (ion)
Proposed struct. shown.
Bis(triphenylphosphine)iminium salt: [92078-18-7].
Synth. from $[(\mu\text{-H})Fe_3(CO)_9BH_3]^{\ominus}$ + CO in toluene at 45° for 2 days. Red-brown cryst. Sol. toluene, Me_2CO.

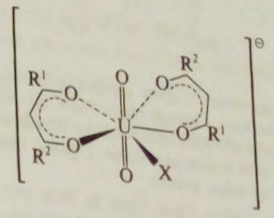
Fehlner, T.P. *et al*, *Organometallics*, 1984, **3**, 1591 (*synth*)
Housecroft, C.E. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 4867 (*synth, ir, pmr, B-11 nmr*)
Jacobsen, G.B. *et al*, *Inorg. Chem.*, 1987, **26**, 4040 (*reaction*)

$C_{10}H_2ClF_{12}O_6U^{\ominus}$

Chlorobis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O*,*O*′)dioxouranate(*VI*)(1 –), 11CI

IC-006682

[83862-68-4]



R^1 = R^2 = CF_3, X = Cl

M 719.5 (ion)
7-Coord. pentagonal bipyramid. Similar compds. formed for X = Br, N_3.
Me_4N salt: [84943-84-0].
Yellow cryst. (CH_2Cl_2). Sol. CH_2Cl_2.

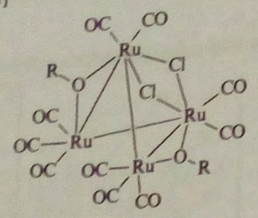
Prasad, L. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 181 (*synth, cryst struct*)
Glavincevski, B. *et al*, *Inorg. Chem.*, 1983, **22**, 221 (*synth, nmr*)

IC-006683

$C_{10}H_2Cl_2O_{12}Ru_4$

Decacarbonyldichlorodihydroxytetraruthenium, 10CI

[63454-09-1]



R = H

M 789.3

A by-product in the reduction of methanolic $RuCl_3.xH_2O$ by CO (10 atm.) in the presence of zinc. Yellow solid. Sol. heptane. Ir ν_{CO} 2093, 2073, 2072, 2070, 2023, 2015, 2011, 1956, 1951 cm^{-1} (heptane).

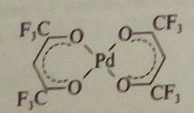
Eady, C.R. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 477 (*synth, ir, ms*)

IC-006684

$C_{10}H_2F_{12}O_4Pd$

Bis(1,1,1,5,5,5-hexafluoropentane-2,4-dionato-*O,O′*) palladium(*II*), 10CI

[64916-48-9]



M 520.5

Square planar struct. Yellow needles (subl.). Large red needles (hexane). Orange plates (MeOH). Sol. many org. solvs. Mp 99.6°. Subl. 50° *in vacuo*. Many studies of reactions with donor molecules. Ligands can be displaced by other anions.

Siedle, A.R. *et al, Inorg. Chem.*, 1980, **19**, 2052; 1981, **20**, 3399; 1983, **22**, 2281 (*synth, cryst struct, ir, ω, pmr, cmr, F-19 nmr, reactions*)

Okeya, S. *et al, Bull. Chem. Soc. Jpn.*, 1981, **54**, 1085 (*synth, ir, pmr, cmr, F-19 nmr*)

Behr, A. *et al, Organometallics*, 1986, **5**, 514 (*reactions*)

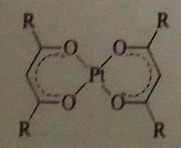
IC-006685

$C_{10}H_2F_{12}O_4Pt$

Bis(1,1,1,5,5,5-hexafluoropentane-2,4-dionato)platinum, 10CI

Bis(hexafluoroacetylacetonato)platinum(II)

[65353-51-7]



R = CF_3

M 609.1

Square planar struct. Ligand known as hfac. Synth. from $[Pt(H_2O)_4]^{2\oplus}$ + Hhfac + $OH^{\ominus}$. Orange needles. Sol. many org. solvs. Subl. 65°.

Inorg. Synth., 1980, **20**, 65 (*synth*)

Okeya, S. *et al, Bull. Chem. Soc. Jpn.*, 1981, **54**, 1085 (*ir, pmr, cmr, F-19 nmr*)

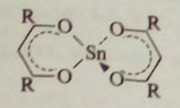
IC-006686

$C_{10}H_2F_{12}O_4Sn$

Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O,O′*)tin, 9CI

Bis(hexafluoroacetylacetonato)tin(II)

[51319-99-4]



R = CF_3

M 532.8

Synth. by reaction of Sn(*II*) compds. with the β-diketone. Glistening white cryst. Subl.$_{0.01}$ 80°.

Ewings, P.F.R. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 821 (*synth, mössbauer, nmr, ms*)

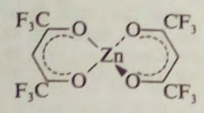
IC-006687

$C_{10}H_2F_{12}O_4Zn$

Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O,O′*)zinc, 9CI

Bis(hexafluoroacetylacetonato)zinc

[14949-70-3]



M 479.4

Cryst. Forms a dihydrate.

[16743-33-2]

Reichert, C. *et al, Can. J. Chem.*, 1970, **48**, 1362 (*ms*)

Yaqub, M. *et al, J. Inorg. Nucl. Chem.*, 1971, **33**, 1944 (*synth, ir*)

Gurevich, M.Z. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1975, **20**, 250 (*synth*)

Dakternicks, D.R. *et al, Aust. J. Chem.*, 1979, **32**, 2405 (*ms*)

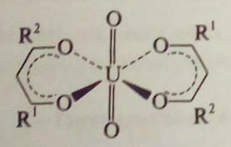
IC-006688

$C_{10}H_2F_{12}O_6U$

Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O,O′*) dioxouranium(*VI*)

Uranyl hexafluoroacetylacetonate

[85647-74-1]



$R^1 = R^2 = CF_3$

M 684.1

Cryst. as trimer. Dimer in gas phase, partly dissociated. Studied for potential in U-isotope separation. Forms adducts with THF, DMSO, $(MeO)_3PO$, H_2O, etc. Ir $\nu_{O=U=O}$ 955, 860 cm^{-1} (vapour).

Trimer: [67761-38-0].

$C_{30}H_6F_{36}O_{18}U_3$ M 2052.3

V. hygroscopic deep red cryst. Mp 183°. Subl. 120° *in vacuo*. 7-Coord. U by bridging of uranyl groups. Ir $\nu_{O=U=O}$ 950, 936, 920 cm^{-1}.

Hydrate (monomeric): Aquabis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-O,O′)dioxouranium(VI)

$C_{10}H_4F_{12}O_7U$ M 702.1

Yellow cryst. Subl.$_{0.001}$ 30-50°. Dec. > 50°.

Ammine complex: [72388-59-1]. *Amminebis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-O,O′)dioxouranium*(VI), *10CI*

Yellow cryst. Subl. 80°. 7-Coord. pentagonal bipyramid.

THF complex: see *Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-O,O′)dioxo(tetrahydrofuran)uranium*(VI), *IC-008532*

[67316-66-9]

Belford, R.L. *et al, J. Inorg. Nucl. Chem.*, 1969, **14**, 169 (*synth*)

Fragala, I. *et al, Inorg. Chem.*, 1978, **17**, 3175 (*synth, pe*)

Taylor, J.C. *et al, Inorg. Chem.*, 1978, **17**, 3285 (*cryst struct*)

Ekstrom, A. *et al, Inorg. Nucl. Chem. Lett.*, 1978, **14**, 301 (*synth*)

Ekstrom, A. *et al, J. Phys. Chem.*, 1978, **82**, 2180 (*vp*)

Kaldov, A. *et al, J. Am. Chem. Soc.*, 1979, **101**, 4465 (*use*)

Kramer, G.M. *et al, Inorg. Chem.*, 1980, **19**, 1340; 1981, **20**, 1415, 1418 (*derivs*)

Maas, E.T. *et al, J. Inorg. Nucl. Chem.*, 1981, **43**, 2053 (*synth, ir, deriv*)

Bray, R.G. *et al, Inorg. Chem.*, 1983, **22**, 1843 (*ir, raman*)

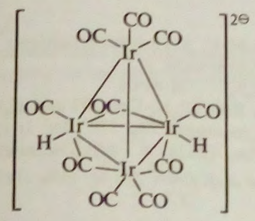
Bray, R.G., *Spectrochim. Acta, Part A*, 1983, **39**, 559 (*ir, raman*)

IC-006689

$C_{10}H_2Ir_4O_{10}^{2\ominus}$

Tri-μ-carbonylheptacarbonyldihydrotetrairidate(2−)

Decacarbonyldihydrotetrairidate(2−)



M 1051.0 (ion)

Bis[bis(triphenylphosphine)iminium] salt: [67388-82-3]. Orange-brown prisms.

Ciani, G. *et al, J. Organomet. Chem.*, 1978, **150**, C17 (*ir, pmr, struct*)

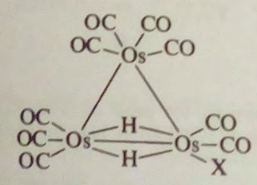
IC-006690

$C_{10}H_2O_{10}Os_3$

Decacarbonyldi-μ-hydrotriosmium, 9CI

1,1,1,1,2,2,2,3,3,3-Decacarbonyl-2,3-dihydrotriosmium

[41766-80-7]



X = CO

M 852.7

Dark-red or intense purple-black cryst. (pentane).

Johnson, B.F.G. *et al, J. Chem. Soc. A*, 1968, 2859 (*synth, ir, pmr, ms*)

Knox, S.A.R. *et al, J. Am. Chem. Soc.*, 1975, **97**, 709.

Orpen, A.G. *et al, J. Chem. Soc., Chem. Commun.*, 1978, 723 (*struct*)

Broach, R.W. *et al, Inorg. Chem.*, 1979, **18**, 314 (*struct*)

Johnson, B.F.G., *Transition Metal Clusters*, Wiley, N.Y., 1980 (*rev*)

Johnson, B.F.G. *et al, Adv. Inorg. Chem. Radiochem.*, 1981, **24**, 225 (*rev*)

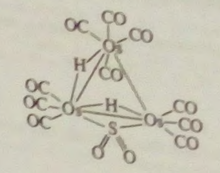
Aime, S. *et al, J. Organomet. Chem.*, 1981, **213**, 207 (*cmr*)

IC-006691

$C_{10}H_2O_{12}Os_3S$

Decacarbonyldi-μ-hydro-μ-sulfonyltriosmium

[91002-40-3]



M 916.7

Yellow cryst. Sol. Me_2CO, sl. sol. CH_2Cl_2, C_6H_6, insol. heptane, THF.

Jarvinen, G.D. *et al, Organometallics*, 1984, **3**, 1434 (*synth, struct, pmr, ir*)

IC-006692

$C_{10}H_3AsCo_2O_9Ru$

Tricarbonyl(hexacarbonyldicobalt)[μ_3-(methylarsinidene)] ruthenium, 11CI

[86272-86-8]

As Tricarbonyl(hexacarbonyldicobalt)-μ_3-thioxoruthenium, IC-006433 with

X = AsMe

M 560.9

Dark-brown cryst. Mp > 250° dec.

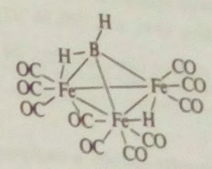
Roland, E. *et al, Organometallics*, 1983, **2**, 1048 (*synth, ir, pmr*)

IC-006693

$C_{10}H_3BFe_3O_{10}$

μ-Boryl-μ-carbonylnonacarbonyl-μ-hydrotriiron

[92055-44-2]



M 461.4

Mod. air-stable brown solid.

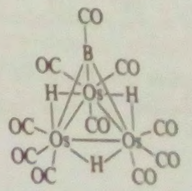
Vites, J.C. *et al, Organometallics*, 1984, **3**, 1591 (*synth, ms, ir, pmr, B-11 nmr*)

IC-006694

$C_{10}H_3BO_{10}Os_3$

[μ_3-(Carbonylboryl)]nonacarbonyltri-μ-hydrotriosmium, 11CI

[86727-98-2]



M 864.5

Bright-yellow air-stable cryst. Subl. 60° *in vacuo*.

Shore, S.G. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 5923 (*synth, ir, pmr, cmr, B-11 nmr*)

IC-006695

$C_{10}H_3Co_2FeO_9P$

Tricarbonyl(hexacarbonyldicobalt)[μ_3-(methylphosphinidene)]iron, 11CI

[87160-19-8]

As Tricarbonyl(hexacarbonyldicobalt)-μ_3-selenoxoiron with

X = PMe

M 471.8

Black powder. Dec. at 165-175°.

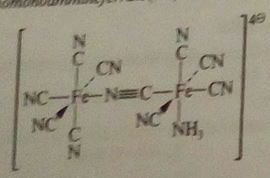
Müller, M. *et al*, *Chem. Ber.*, 1983, **116**, 2311 (*synth, pmr, ir*)

IC-006696

$C_{10}H_3Fe_2N_{11}^{4\ominus}$

Ammine[-μ-(cyano-*C*:*N*)]nonakis(cyano-*C*)diferrate(*III*) (4−), 11CI

Pentacyanoferrate(III)-μ-cyano-tetracyanomonoammineferrate(III)



M 388.9 (ion)

Bioctahedral. Synth. from $[Fe(CN)_6]^{3\ominus}$ and $[Fe(CN)_5(NH_3)]^{2\ominus}$. Exhibits antiferromagnetic coupling between Fe(*III*) centres via $CN^{\ominus}$ bridge.

Tetrakis-Ph$_4$P salt: [70700-82-2].

Obt. by air oxidn. of aq. solns. of $Na_4[Fe(CN)_5(NH_3)].3H_2O$ followed by cation exchange. Dark green cryst. + $6H_2O$ (aq.EtOH) which dissolve in H_2O or EtOH to give a purple soln. Sol. H_2O, EtOH. Dimer-monomer equilm., in soln.

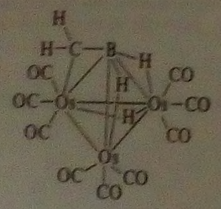
Rieder, P. *et al*, *Inorg. Chim. Acta*, 1979, **34**, 113 (*struct, mössbauer*)

Michaels, L.P. *et al*, *Inorg. Chim. Acta*, 1985, **100**, 211 (*synth, struct, magnetism, ir, us-vis*)

$C_{10}H_3BO_9Os_3$ IC-006697

(Boron)nonacarbonyltri-μ-hydro-μ-methylenetriosmium, 11CI

[106469-32-3]



M 850.5

Air-stable pale-yellow cryst. (Et_2O). Sol. hexane.

Jan, D.-Y., *Organometallics*, 1987, **6**, 428 (*synth, ms, ir, cryst struct, pmr, B-11 nmr*)

$C_{10}H_5N_5S_5Ta$ IC-006698

(Pyridine)pentakis(thiocyanato-*N*)tantalum(*V*), 9CI

Pentakis(isothiocyanato)(pyridine)tantalum(V), *8CI*

[16918-27-7]

$PyTa(NCS)_5$

M 550.4

Octahedral around Ta. Synth. from Hexakis(thiocyanato-*N*)tantalate(*V*)(1−), IC-005625 and excess Py or from $TaCl_5$, KNCS and Py in MeCN. Light brown solid. Sol. MeCN; insol. CH_2Cl_2. Mp 130° dec.

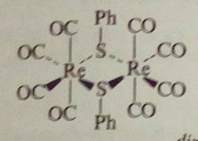
Boehland, H. *et al*, *J. Less-Common Met.*, 1967, **13**, 224 (*synth, ir, us-vis*)

Smith, J.N. *et al*, *Inorg. Chem.*, 1972, **11**, 2697 (*synth, ir, us-vis*)

$C_{10}H_5O_4ReS$ IC-006699

(Benzenethiolato)tetracarbonylrhenium

Tetracarbonyl(phenylthio)rhenium



dimer

M 407.4

Dimeric.

Dimer: [15680-94-1]. *Bis(μ-benzenethiolato) octacarbonyldirhenium, 8CI*

$C_{20}H_{10}O_8Re_2S_2$ M 814.8

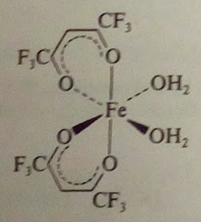
Synth. from $Re(CO)_5H$, C_6H_5SH and C_6H_6. Pale-yellow cryst. (C_6H_6/pentane). Mp 270° dec. Ir ν_{CO} 2100m, 2022vs, 1995m, 1962s cm^{-1} (cyclohexane).

Osborne, A.G. *et al*, *J. Chem. Soc. A*, 1966, 1143 (*synth, ir*)

$C_{10}H_6F_{12}FeO_6$ IC-006700

Diaquabis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O*,*O*′)iron(*II*), 11CI

[64146-52-7]



M 505.9

Octahedral. Intermed. for prep. of $[FeL_2X_2]$ complexes. Synth. from $FeSO_4.7H_2O$ + NaL in H_2O. Red brown solid.

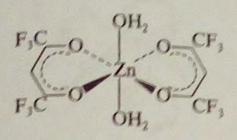
Bailey, N.A. *et al*, *Inorg. Chim. Acta*, 1984, **88**, 125 (*synth, ir, mössbauer*)

$C_{10}H_6F_{12}O_6Zn$ IC-006701

Diaquabis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O*,*O*′)zinc(*II*)

Bis(hexafluoroacetylacetonato)zinc(II) *dihydrate*

[16743-33-2]



M 515.5

trans-Octahedral struct. Monomeric in EtOH soln. Cryst. (aq. EtOH or $CHCl_3$). Sol. MeOH, EtOH, Me_2CO, Et_2O; insol. H_2O, CCl_4. Mp 153-154°. Subl. 50°. Dehydrates to Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O*,*O*′)zinc, IC-006687 on heating *in vacuo* over P_2O_5.

[42087-52-5, 106293-68-9]

Morris, M.L. *et al*, *Inorg. Chem.*, 1963, **2**, 411 (*synth, ir*)

Chattoraj, S.C. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1937 (*synth, ir, pmr*)

Kidd, M.R. *et al*, *Inorg. Chem.*, 1967, **6**, 946 (*synth*)

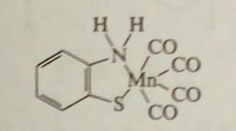
Gurevich, M.Z. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1975, **20**, 250 (*synth, thermal stability*)

Adams, R.P. *et al*, *Inorg. Chim. Acta*, 1986, **119**, 67 (*cryst struct*)

$C_{10}H_6MnNO_4S$ IC-006702

(2-Aminobenzenethiolato)tetracarbonylmanganese

(o-Aminophenylthio)tetracarbonylmanganese



M 291.1

Synth. from $MnBr(CO)_5$ and *o*-$H_2NC_6H_4SH$. Light-yellow needles. Ir ν_{CO} 2021s, 1928vs, 1902vs, 1889vs cm^{-1} (KBr).

Hieber, W. *et al*, *Chem. Ber.*, 1966, **99**, 2312 (*synth, ir*)

$C_{10}H_6Mn_2O_8S_2$ IC-006703

Octacarbonylbis[μ-(methanethiolato)]dimanganese, 10CI

[21321-38-0]

As Octacarbonylbis[μ-(trifluoromethanethiolato)] dimanganese, IC-006673 with

R = Me

M 428.1

Synth. from $HMn(CO)_5$ and MeSSMe. Yellow-orange cryst. (pentane). Ir ν_{CO} 2095w, 2074s, 2016vs, 2002vs, 1985m, 1969s, 1937w cm^{-1} (cyclohexane). Dec. at 120° without melting.

Monomer:

$C_5H_3MnO_4S$ M 214.0

Has no separate existence.

Treichel, P.M. *et al*, *J. Chem. Soc.*, 1963, 720 (*synth, ir*)

Osborne, A.G. *et al*, *J. Chem. Soc. A*, 1966, 1143 (*synth, ir*)

Küllmer, V. *et al*, *Chem. Ber.*, 1977, **110**, 228 (*synth*)

$C_{10}H_6Mn_2O_8Se_2$ IC-006704

Octacarbonylbis[μ-(methaneselenolato)]dimanganese, 9CI

Bis(methaneselenolato)octacarbonyldimanganese

[15748-45-5]

As Octacarbonyldi-μ-selenyldimanganese, IC-005890 with

R = Me

M 521.9

Synth. from $HMn(CO)_5$ and Me_2Se_2. Orange-red cryst. (pentane). Mp 160° dec. (110° dec.). Ir ν_{CO} 2050vs, 2010vs, 1985vs, 1970vs, 1950vs cm^{-1} (KBr); 2058s, 2003vs, 2000vs, 1993s, 1960vs cm^{-1} (cyclohexane).

Welcman, N. *et al*, *J. Chem. Soc.*, 1965, 7515 (*synth, ir, pmr*)

Abel, E.W. *et al*, *J. Chem. Soc. A*, 1967, 2014 (*synth, ir, pmr*)

Küllmer, V. *et al*, *Chem. Ber.*, 1977, **110**, 228 (*synth*)

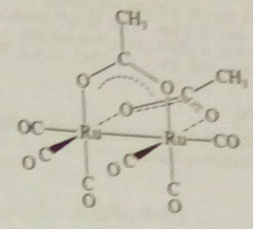
Grobe, J. *et al*, *J. Fluorine Chem.*, 1978, **11**, 265 (*synth, ir, pmr*)

$C_{10}H_4O_{10}Ru_2$

Bis[μ-(acetato-*O*:*O*′)]hexacarbonyldiruthenium, 9CI IC-006705

Di-μ-ethanoato-(O,O′)-bis[tricarbonylruthenium(I)]

[24846-19-3]



M 488.2

Prepd. by treating (Acetato-*O*)dicarbonylruthenium, IC-003920 in hexane with CO (50 atm.; 80°) or by reduction of $RuCl_3.xH_2O/H_2O/AcOH/NaOAc$ with CO (1 atm.; 80°). Pale yellow cryst.; unstable, loses CO *in vacuo* or in soln. at r.t. to give (Acetato-*O*) dicarbonylruthenium, IC-003920. Sol. hexane. Ir ν_{CO} 2106, 2098, 2082, 2038, 2008, 1944 cm^{-1} (hexane).

Crooks, G.R. *et al*, *J. Chem. Soc. A*, 1969, 2761 (*synth, ir, pmr*)

James, B.R. *et al*, *Chem. Ind.* (*London*), 1971, 1036 (*synth*)

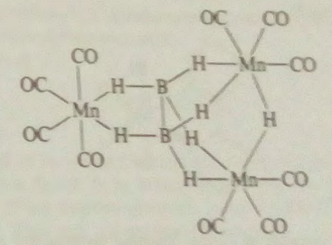
Spohn, M. *et al*, *Z. Naturforsch., B*, 1986, **41**, 1373 (*cryst struct, synth*)

$C_{10}H_7B_2Mn_3O_{10}$ IC-006706

Decacarbonyl(μ$_3$-diborane)-μ-hydrotrimanganese

Hydrobis(borane)decacarbonyltrimanganese

[20982-73-4]



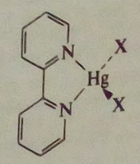
M 473.5

Mn in approx. octahedral environment. Dark red mod. air-stable cryst. (cyclohexane/methylcyclohexane 4:1). Air-sensitive in soln.

Kaesz, H.D. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 2753 (*cryst struct, props, pmr, synth, ir*)

IC-006707

$C_{10}H_8Br_2HgN_2$
(2,2′-Bipyridine-*N*,*N*′)dibromomercury, 11Cl
(2,2′-Bipyridine)mercury dibromide
[72608-73-2]



X = Br

M 516.5
Cryst. Mp 286-289°.
[72608-74-3]

Hein, F. *et al*, *Ber., B*, 1935, **68**, 681 (*synth*)
Sutton, G.J., *Aust. J. Chem.*, 1959, **12**, 637 (*synth, conduct, uv*)
Coates, G.E. *et al*, *J. Chem. Soc.*, 1964, 166 (*ir*)
Zueva, A.N. *et al*, *Uzb. Khim. Zh.*, 1982, 11; *CA*, **97**, 153317 (*ir*)

IC-006708

$C_{10}H_8Br_2MnN_2$
(2,2′-Bipyridine-*N*,*N*′)dibromomanganese(*II*), 11Cl
Dibromobipyridylmanganese(II)
[32425-37-9]

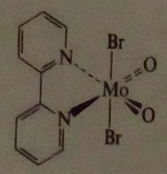
$[MnBr_2(Bipy)]_n$

M 370.9
Assumed to be polymeric octahedal with bridging bromine. Obt. from $MnCl_2$ and bipy in dry Me_2CO. Pale yellow solid which does not dec. or oxidise on heating. Spar. sol. org. solvs. μ_{eff} = 5.82μ_B (298K).

Syamal, A., *J. Indian Chem. Soc.*, 1967, **44**, 989 (*magnetism, struct*)
Strukl, J.S. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 223 (*synth, ir*)
Wilde, R.E. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1017; 1974, **36**, 323 (*synth, ir, raman*)
Ahuja, I.S. *et al*, *J. Mol. Struct.*, 1981, **74**, 143 (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 211 (*rev, bibl*)

IC-006709

$C_{10}H_8Br_2MoN_2O_2$
(2,2′-Bipyridine)dibromodioxomolybdenum(*VI*), 8Cl
2,2′-Bipyridyldibromodioxomolybdenum(VI)
[25411-14-7]

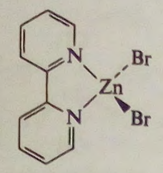


M 443.9
Distorted octahedral config. Starting material for other Mo complexes. Yellow cryst.

Hull, C.G. *et al*, *J. Chem. Soc. A*, 1966, 1633 (*synth, ir*)
Fenn, R.H., *J. Chem. Soc. A*, 1969, 1764 (*cryst struct*)
Schrauzer, G.N. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 4760 (*reactions*)
Ross, F. *et al*, *Organometallics*, 1983, **2**, 481 (*reactions*)

IC-006710

$C_{10}H_8Br_2N_2Zn$
(2,2′-Bipyridine-*N*,*N*′)dibromozinc(*II*), 9Cl
(2,2′-Bipyridine)zinc dibromide
[14324-78-8]

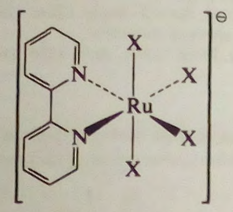


M 381.3
Colourless cryst. ($PhNO_2$). Sol. toluene. Mp >360°.

Coates, G.E. *et al*, *J. Chem. Soc.*, 1964, 166 (*synth, ir*)
Noltes, J.G. *et al*, *J. Organomet. Chem.*, 1965, **3**, 222 (*synth, uv*)
Postmus, C. *et al*, *Inorg. Chem.*, 1967, **6**, 2030 (*ir*)
Strukl, J.S. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 223 (*ir, raman*)
Alyaviya, M.K. *et al*, *Koord. Khim.*, 1975, **1**, 190 (*pmr*)

IC-006711

$C_{10}H_8Br_4N_2Ru^{\ominus}$
(2,2′-Bipyridine-*N*,*N*′)tetrabromoruthenate(*III*)(1−), 9Cl



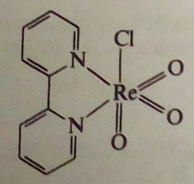
X = Br

M 576.8 (ion)
K salt: [31296-54-5].

Dwyer, F.B. *et al*, *Aust. J. Chem.*, 1963, **16**, 42 (*synth*)
Bryant, G.M. *et al*, *Aust. J. Chem.*, 1971, **24**, 275 (*synth, uv*)

IC-006712

$C_{10}H_8ClN_2O_3Re$
(2,2′-Bipyridine-*N*,*N*′)chlorotrioxorhenium(*VII*), 10Cl
(Bipyridyl)chlorotrioxorhenium(VII). *Trioxochloro-2,2′-dipyridylrhenium*(VII)
[57526-16-6]

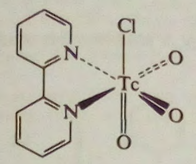


M 425.8
Presumed octahedral, detailed geometry not established. Synth. from ReO_3Cl and bipy in dry CCl_4 or from $NaReO_4$, aq. HCl and bipy in EtOH. Pale yellow or white solid. Mp 280° dec.

Guest, A. *et al*, *Can. J. Chem.*, 1971, **49**, 603 (*synth, ir, props*)
Sergienko, V.S. *et al*, *Koord. Khim.*, 1977, **3**, 1060.
Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 4300 (*synth, ir, props*)

IC-006713

$C_{10}H_8ClN_2O_3Tc$
Trioxochloro(2,2′-bipyridine-*N*,*N*′)technetium(*VII*), 10Cl
[78939-76-1]

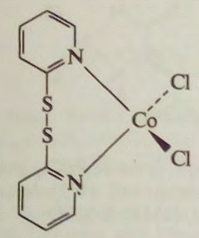


M 338.5
Probably 3 oxygens are facial, struct. not determined. Synth. from $TcO_4^{\ominus}$ plus bipy and conc. HCl in EtOH. Converts alkenes into glycols. Bright yellow solid, hydrol. readily to $TcO_4^{\ominus}$, readily reduced to Tc(*V*) species $TcOCl_3$(bipy). Spar. sol. Me_2CO, CH_2Cl_2, MeCN; insol. toluene, MeOH, EtOH. Mp 162° dec. Analogous complexes exist with phen. and several substituted phen. ligands in place of bipy. Ir $\nu_{Tc=O}$ 905s, 885s, 865m cm^{-1} (KBr).

Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 4300 (*synth, uv, ir, analogues*)
Pearlstein, R.M. *et al*, *Polyhedron*, 1988, **7**, 1981 (*reaction with alkenes*)

IC-006714

$C_{10}H_8Cl_2CoN_2S_2$
[Bis(2-pyridyl) disulfide]dichlorocobalt(*II*)
*Dichloro(2,2′-dithiobis[pyridine]-*N,N′*)cobalt*(II), *9Cl*
[12705-55-4]

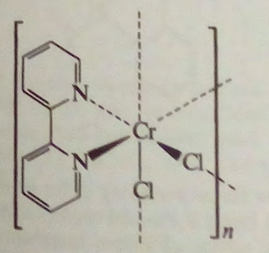


M 350.1
Tetrahedral. Blue cryst. Sol. EtOH. Paramagnetic.

Keeton, M. *et al*, *Inorg. Chem.*, 1971, **10**, 47 (*synth, ir, uv*)
Ferraro, J.R. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 231 (*synth, ir, magnetism*)
Kadooka, M.M. *et al*, *Inorg. Chem.*, 1976, **15**, 812 (*synth, cryst struct, ir, uv*)

IC-006715

$C_{10}H_8Cl_2CrN_2$
(2,2′-Bipyridine-*N*,*N*′)dichlorochromium(*II*), 10Cl
(2,2′-Bipyridyl)dichlorochromium(II)
[66059-28-7]



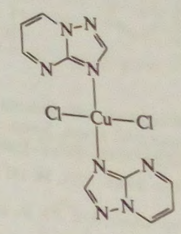
M 279.0

6-Coordinate, polymeric through chloride bridges. Synth. from $CrCl_3.4H_2O$ + bipy in EtOH. Air-sensitive dark brown solid. Sol. H_2O dec. Corresp. dibromide also reported. μ_{eff} = 4.19 (295K); 3.60μ_B (90K).

Lux, H. *et al*, *Chem. Ber.*, 1964, **97**, 503.
Earnshaw, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2209 (*synth, uv, magnetism*)

IC-006716

$C_{10}H_8Cl_2CuN_8$
Dichlorobis([1,2,4]triazolo[1,5-*a*]pyrimidine-*N*³)copper(*II*)
[110693-76-0]

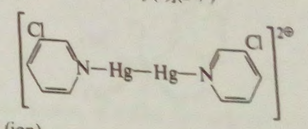


M 374.6
Prismatic blue cryst. (EtOH).

Cingi, M.B. *et al*, *Inorg. Chim. Acta*, 1987, **129**, 217 (*synth, cryst struct, ir, esr*)

IC-006717

$C_{10}H_8Cl_2Hg_2N_2^{2\oplus}$
Bis(3-chloropyridine)dimercury(*I*)(2+), 9Cl
Bis[(3-chloropyridine)mercury(I)](2+)



M 628.2 (ion)
Diperchlorate: [41637-04-1].
Needles (MeOH/ethyl orthoformate/Et_2O). Mp 260-261°.
[53112-87-1]

Kepert, D.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 893 (*synth, cryst struct*)

IC-006718

$C_{10}H_8Cl_2MnN_2$
(2,2′-Bipyridine-*N*,*N*′)dichloromanganese(*II*), 11Cl
Dichlorobipyridylmanganese(II)
[41078-94-8]

$[MnCl_2(Bipy)]_n$

M 282.0
Assumed to be polymeric octahedral with bridging chlorine. Synth. from $MnCl_2$ and Bipy in dry Me_2CO. Pale yellow hygroscopic solid. Insol. EtOH, DMF, Et_2O. High spin manganese(*II*) complex. Disproportionates in H_2O and MeOH.

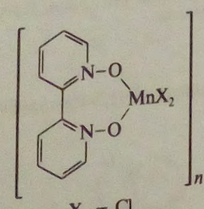
Broomhead, J.A. *et al*, *Aust. J. Chem.*, 1961, **14**, 250 (*synth, magnetism*)
Syamal, A., *J. Indian Chem. Soc.*, 1967, **44**, 989 (*synth, magnetism*)
Strukl, J.S. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 223 (*synth, ir*)
Wilde, R.E. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1017; 1974, **36**, 323 (*synth, ir, raman*)
Ahuja, I.S. *et al*, *J. Mol. Struct.*, 1981, **74**, 143 (*uv, struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 211 (*rev, bibl*)

$C_{10}H_8Cl_2MnN_2O_2$ IC-006719

(2,2′-Bipyridine 1,1′-dioxide-*O,O′*)dichloromanganese(*II*), 11Cl

*Dichloro(bipyridyl-*N,N′*-dioxide)manganese*(II)

[78913-94-7]



X = Cl

M 314.0

Polymeric octahedral struct. with bidentate bipyridyl-*N,N′*-dioxide and bridging Cl atoms. Synth. from ligand and $MnCl_2$ in hot EtOH. Stable in air. Insol. EtOH.

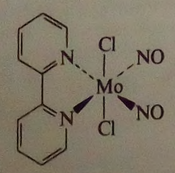
Ahuja, I.S. *et al*, *J. Mol. Struct.*, 1981, **74**, 143 (*synth, magnetism, uv, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 230 (*rev, bibl*)

$C_{10}H_8Cl_2MoN_4O_2$ IC-006720

(2,2′-Bipyridine-*N,N′*)dichlorodinitrosylmolybdenum, 11Cl, 10Cl, 9Cl

Dichlorobis(nitrosyl)-2,2′-bipyridylmolybdenum

[53956-09-5]



M 383.0

Octahedral. Homogeneous olefin disproportionation catalyst; epoxidation catalyst. Yellow-green cryst.

[14324-79-9, 83057-58-3]

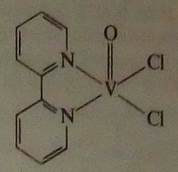
Hughes, W.B. *et al*, *Adv. Chem. Ser.*, 1974, **132**, 192 (*uses*)
Fleischer, J. *et al*, *J. Prakt. Chem.*, 1977, **319**, 995 (*uses*)
Ballivet-Tkatchenko, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 1137 (*cryst struct, synth, ir*)
Ballivet-Tkatchenko, D. *et al*, *Inorg. Chem.*, 1986, **25**, 826 (*electrochem*)

$C_{10}H_8Cl_2N_2OV$ IC-006721

(2,2′-Bipyridine-*N,N′*)dichlorooxovanadium(*IV*), 11Cl

(α,α′-Bipyridyl)dichlorooxovanadium(IV)

[52595-68-3]



M 294.0

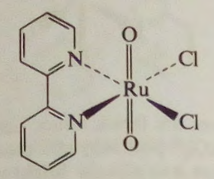
Synth. by adding bipy in Et_2O to $VOCl_2$.3MeOH in Et_2O or by recrystallising VCl_4(bipy) from a moist solv. Yellow-green solid. Paramagnetic; μ_{eff} = 1.74μ_B (295K).

Clark, R.J.H., *J. Chem. Soc.*, 1963, 1377 (*synth, uv-vis, ir*)
Fowles, G.W.A. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 642 (*synth, uv-vis, ir*)

$C_{10}H_8Cl_2N_2O_2Ru$ IC-006722

(2,2′-Bipyridine-*N,N′*)dichlorodioxoruthenium(*VI*), 9Cl

[42769-04-0]



M 360.1

Approx. octahedral. Prepd. by treating RuO_4 in CCl_4 with mildly basic [bipyH]Cl at 0°. Mild oxidant for unsaturated alcohols. Yellow, diamagnetic solid. Ir ν_{RuO_2} 839 cm^{-1}.

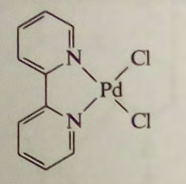
Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)
Green, G. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1984, 681 (*use*)

$C_{10}H_8Cl_2N_2Pd$ IC-006723

(2,2′-Bipyridine-*N,N′*)dichloropalladium(*II*), 9Cl

(2,2′-Bipyridyl)dichloropalladium(II)

[14871-92-2]



M 333.5

Square planar. Synth. from K_2PdCl_4 and bipy with heating. Yellow cryst. (dil. HCl). Insol. cold H_2O; mod. sol. hot H_2O; sol. DMF, DMSO.

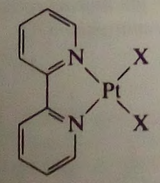
Inorg. Synth., 1971, **13**, 216.
Gidney, P.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 185 (*uv*)
Norbury, A.H. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1211 (*ir*)

$C_{10}H_8Cl_2N_2Pt$ IC-006724

(2,2′-Bipyridine-*N,N′*)dichloroplatinum, 8Cl

(2,2′-Bipyridyl)dichloroplatinum(II). *(2,2′-Dipyridyl)dichloroplatinum*(II)

[13965-31-6]



X = Cl

M 422.1

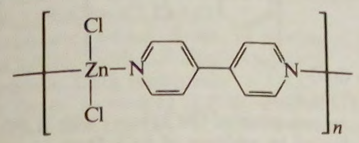
Red and yellow forms probably differ in molecular packing, red being a stacked struct. with anisotropic uv-vis spectrum; struct. of yellow form not reported. Many mechanistic studies of substitutions undertaken. Yellow cryst. (H_2O); red cryst. (aq. HCl). Sol. polar org. solvs; spar sol. $CHCl_3$, CH_2Cl_2.

Morgan, G.T. *et al*, *J. Chem. Soc.*, 1934, 965 (*synth*)
Strukl, J.S. *et al*, *Spectrochim. Acta, Part A*, 1971, **27**, 223 (*ir*)
Gidney, P.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 132 (*uv*)
Clark, D.T. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 169 (*nqr, pe*)
Norbury, A.H. *et al*, *J. Inorg. Nucl. Chem.*, 1973, **35**, 1211 (*ir*)
Osborn, R.S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 1002 (*struct*)
Beilli, E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2133 (*synth, ir, pmr, uv*)
Marcelis, A.J.M. *et al*, *Inorg. Chim. Acta*, 1983, **78**, 195 (*pmr*)
Hope, E.G. *et al*, *Inorg. Chim. Acta*, 1986, **115**, 187 (*Pt-195 nmr*)

$C_{10}H_8Cl_2N_2Zn$ IC-006725

(4,4′-Bipyridine)dichlorozinc

[26678-77-3]



tentative struct.

M 292.4

Probably polymeric in the solid state. Solid (H_2O). Indexed as a dimer in CA.

Ferraro, J.R. *et al*, *Inorg. Chim. Acta*, 1969, **3**, 685 (*synth, ir*)

$C_{10}H_8Cl_3CrN_2O$ IC-006726

(2,2′-Bipyridine-*N,N′*)trichlorooxochromium(*V*), 9Cl

2,2′-Bipyridyltrichlorooxochromium(V)

[54184-21-3]

$(Bipy)CrOCl_3$

M 330.5

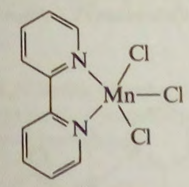
Struct. not fully descr. Brown air-stable cryst. Insol. H_2O, common solvs., sl. sol. Me_2CO, dec. aq. alkalis. Paramagnetic; μ_{eff} = 1.85μ_B (297K).

Sarkar, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1974, 509.
Seddon, E.A. *et al*, *Transition Met. Chem.*, 1978, **3**, 318 (*synth*)
Edwards, D.A. *et al*, *Transition Met. Chem.*, 1981, **6**, 235.
Saha, H.K. *et al*, *J. Indian Chem. Soc.*, 1983, **60**, 599.
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 934 (*rev*)

$C_{10}H_8Cl_3MnN_2$ IC-006727

(2,2′-Bipyridine-*N,N′*)trichloromanganese(*III*), 9Cl

[31287-68-0]



M 317.4

Assumed to be dimeric. Synth. by thermal dec. of [bipyH$_2$]$MnCl_5$ at 100° for 90 min. or from $MnCl_3$ and bipy in Et_2O. Air-stable dark red leaflets. Insol. Et_2O; sl. sol. (with dec.) Me_2CO, $MeNO_2$. Dec. above 180°. μ_{eff} = 4.25μ_B (292K).

*Dimer: Tetrakis(2,2′-bipyridine-*N,N′*)di-μ-chlorodichlorodimanganese*(III)
$C_{20}H_{16}Cl_6Mn_2N_4$ M 634.9

Monohydrate (monomeric): [15632-12-9]. *Aqua(2,2′-bipyridine-*N,N′*)trichloromanganese*(III), *10Cl*

$C_{10}H_{10}Cl_3MnN_2O$ M 335.4

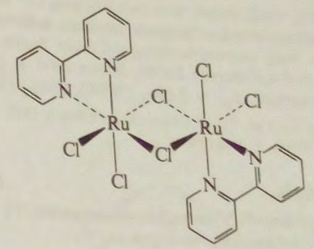
Synth. from $KMnO_4$, 10*M* HCl + bipy. Catalyses oxidation of isopropylbenzene by O_2 at 70°. Purple-brown solid. Loses H_2O on heating in air between 65-110°. Octahedral geometry proposed. μ_{eff} = 4.98 μ_B (288K).

Goodwin, H.A. *et al*, *Aust. J. Chem.*, 1965, **18**, 1743; 1967, **20**, 629 (*magnetism, synth, uv, hydrate*)
Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1967, **349**, 45 (*thermal dec*)
Sychev, A.Ya. *et al*, *Russ. J. Phys. Chem.* (*Engl. Transl.*), 1969, **43**, 370 (*props*)
Ghosh, S.N., *J. Inorg. Nucl. Chem.*, 1972, **34**, 1456 (*ir, hydrate*)
Akabori, K., *Chem. Lett.*, 1974, 1481 (*magnetism*)
Bell, C.F. *et al*, *J. Inorg. Nucl. Chem.*, 1977, **39**, 773 (*synth, hydrate, ir, raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 219 (*rev, bibl*)

$C_{10}H_8Cl_3N_2Ru$ IC-006728

(2,2′-Bipyridine-*N,N′*)trichlororuthenium(*III*)

[69141-04-4]



dimer

M 363.6

Struct. not known, although probably dimeric. Once incorrectly described as (2,2′-Bipyridine-*N,N′*) tetrachlororuthenium(*IV*), IC-006736. Prepd. either by treating $RuCl_3.xH_2O$ in 1*M* HCl with 2,2′-bipy, or by reducing (2,2′-Bipyridine-*N,N′*)tetrachlororuthenium(*IV*), IC-006736 with HCl/EtOH, followed by heating at 180°. Useful synthetic reagent. Brown powder. Insol.

Dimer:
$C_{20}H_{16}Cl_6N_4Ru_2$ M 727.2

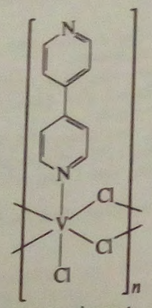
Dwyer, F.P. *et al*, *Aust. J. Chem.*, 1963, **16**, 42 (*synth*)
Krause, R.A., *Inorg. Chim. Acta*, 1977, **22**, 209 (*synth*)
Anderson, S. *et al*, *J. Chem. Res.* (*S*), 1979, 74 (*synth, reaction*)
Belser, P. *et al*, *Inorg. Chem.*, 1981, **20**, 3098 (*reaction*)
Steel, P.J. *et al*, *Inorg. Chem.*, 1983, **22**, 1488 (*reaction*)
Thummel, R.P. *et al*, *Inorg. Chem.*, 1987, **26**, 3072 (*reaction*)
Lever, A.B.P. *et al*, *J. Am. Chem. Soc.*, 1988, **110**, 8076 (*reaction*)
Campagna, S. *et al*, *Gazz. Chim. Ital.*, 1989, **119**, 415 (*reaction*)

$C_{10}H_8Cl_3N_2V$ IC-006729

(4,4′-Bipyridine-*N*)trichlorovanadium(*III*), 11Cl

(γ,γ′-Bipyridyl)trichlorovanadium(III)

[88641-91-2]



Proposed struct.

M 313.4

Polymeric chain struct. with two bridging $Cl^{\ominus}$ as shown is consistent with low magnetic moment; authors suggest a struct. with unusual bridging 4,4′-bipy. Synth. from VCl_3 and 4,4′-bipy in EtOH. Brown solid + $1H_2O$. Paramagnetic; $\mu_{eff} = 0.89\mu_B$ (285K), $0.86\mu_B$ (100K).

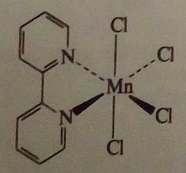
Karwecka, Z. *et al*, *Pol. J. Chem.* (*Rocz. Chem.*), 1982, **56**, 601 (*synth, uv-vis, ir, magnetism*)

$C_{10}H_8Cl_4MnN_2$ IC-006730

(2,2′-Bipyridine-*N,N′*)tetrachloromanganese(*IV*)

(2,2′-Bipyridyl)tetrachloromanganese(IV)

[17084-12-7]



M 352.9

Synth. by adding $KMnO_4$ in 10*M* HCl to a soln. of bipy in 5*M* HCl. Black cryst. (conc. aq. HCl). $\mu_{eff} = 3.82\mu_B$ (291K). Loses Cl_2 at r.t. At 150-155° dec. to $[MnCl_3(bipy)]_2$.

Goodwin, H.A. *et al*, *Aust. J. Chem.*, 1965, **18**, 1743; 1967, **20**, 629 (*synth, props, magnetism*)

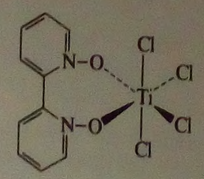
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 225 (*rev, bibl*)

$C_{10}H_8Cl_4N_2O_2Ti$ IC-006731

(2,2′-Bipyridine 1,1′-dioxide-*O,O′*) tetrachlorotitanium(*IV*), 11Cl

Titanium(IV) *chloride 2,2′-bipyridyl*-N,N′-*dioxide*

[85625-97-4]



M 377.8

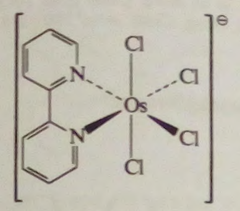
Synth. by mixing C_6H_6 solns. of $TiCl_4$ and bipy-O_2. White solid. Insol. C_6H_6, Et_2O. Mp >250°.

Srivastava, P.C. *et al*, *J. Indian Chem. Soc.*, 1983, **60**, 14 (*synth, ir*)

$C_{10}H_8Cl_4N_2Os^{\ominus}$ IC-006732

(2,2′-Bipyridine-*N,N′*)tetrachloroosmate(*III*)(1−)

[116863-23-1]



M 488.1 (ion)

K salt: [31296-61-4].

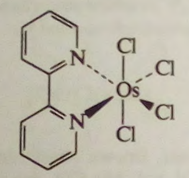
Synth. by reduction of $OsCl_4$(bipy) with H_3PO_2 in 2*M* HCl followed by addition of KCl. Dark brown cryst.

Buckingham, D.A. *et al*, *Aust. J. Chem.*, 1964, **17**, 320 (*synth*)
Bryant, G.M. *et al*, *Aust. J. Chem.*, 1971, **24**, 275 (*uv*)
Kober, E.M. *et al*, *Inorg. Chem.*, 1988, **27**, 4587 (*electrochem, uv*)

$C_{10}H_8Cl_4N_2Os$ IC-006733

(2,2′-Bipyridine)tetrachloroosmium(*IV*), 11Cl

[57288-05-8]



M 488.1

Synth. by pyrolysis of $(bipyH_2)[OsCl_6]$ at 295° for 1h., followed by reflux with H_3PO_2 in 2*M* HCl. Then bubble through Cl_2. Starting material for other osmium bipy complexes. Orange-brown cryst.

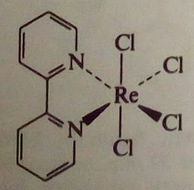
Buckingham, D.A. *et al*, *Aust. J. Chem.*, 1964, **17**, 315 (*synth, use*)
Sullivan, P.B. *et al*, *Organometallics*, 1984, **3**, 1241 (*use*)
Kober, E.M. *et al*, *Inorg. Chem.*, 1988, **27**, 4587 (*use*)

$C_{10}H_8Cl_4N_2Re$ IC-006734

(2,2′-Bipyridine-*N,N′*)tetrachlororhenium(*IV*), 11Cl

Tetrachloro(bipyridyl)rhenium(IV). *Rhenium*(IV) *chloride bipyridine*

[17099-98-8]



M 484.2

Synth from Tetrachlorobis(pyridine)rhenium(*IV*), IC-006813 and bipy or by pyrolysis of $(bipyH_2)ReCl_6$ at 330-350°. Crystalline brownish-yellow powder.

Tronev, V.G., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 1351 (*synth, props, struct*)
Caspar, J.V. *et al*, *Inorg. Chem.*, 1984, **23**, 2104 (*props*)

$C_{10}H_8Cl_4N_2Ru^{\ominus}$ IC-006735

(2,2′-Bipyridine-*N,N′*)tetrachlororuthenate(*III*)(1−), 9Cl

[99949-19-6]

As (2,2′-Bipyridine-*N,N′*)tetrabromoruthenate(*III*)(1−), IC-006711 with

X = Cl

M 399.0 (ion)

K salt: Synth. by treating (2,2′-Bipyridine-*N,N′*) tetrachlororuthenium(*IV*), IC-006736 with HCl/EtOH, followed by KCl in HCl. Brown solid.

Diaqua(2,2′-bipyridine)dichlororuthenium(III)(1+) *salt:* Synth. by treating $K[Ru(bipy)Cl_4]$ with aq. H_2SO_4. Dark brown solid + $2H_2O$. Formulated as $[Ru(bipy)Cl_2(OH_2)_2][Ru(bipy)Cl_4].2H_2O$.

2,2′-Bipyridinium(1+) salt: Synth. by treating $K_2[RuCl_5(OH_2)]$ with 2,2′-bipy. in aq. HCl. Anthelmintic. Dark brown solid + $1H_2O$. $\mu_{eff} = 2.31\mu_B$.

NH_4 salt: Synth. by treating (2,2′-Bipyridine-*N,N′*) tetrachlororuthenium(*IV*), IC-006736 with HCl/EtOH, followed by $[NH_4]Cl$ in aq. HCl. Yellow salt.

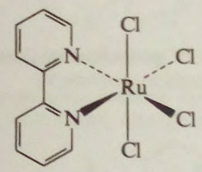
Dwyer, F.B. *et al*, *Aust. J. Chem.*, 1963, **16**, 42 (*synth*)
Figgis, B.N. *et al*, *J. Chem. Soc. A*, 1966, 422 (*magnetism*)
Bryant, G.M. *et al*, *Aust. J. Chem.*, 1971, **24**, 275 (*synth, uv*)
James, B.R. *et al*, *Inorg. Nucl. Chem. Lett.*, 1975, **11**, 837 (*synth*)

$C_{10}H_8Cl_4N_2Ru$ IC-006736

(2,2′-Bipyridine-*N,N′*)tetrachlororuthenium(*IV*), 9Cl

Ruthenium(IV) *chloride 2,2′-bipyridine*

[63338-26-1]



M 399.0

Proposed octahedral struct. shown. Synthetic reagent. Hydrol. in hot H_2O to give a violet soln.

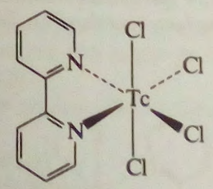
Monohydrate: Prepd. by oxidising a suspension of $[bipyH][Ru(bipy)Cl_4]$ in aq. HCl with Cl_2. $\mu_{eff} = 2.87\mu_B$.

Figgis, B.N., *J. Inorg. Nucl. Chem.*, 1958, **8**, 476 (*magnetism*)
Dwyer, F.P. *et al*, *Aust. J. Chem.*, 1963, **16**, 42 (*synth*)
Takeuchi, K.J. *et al*, *Inorg. Chem.*, 1984, **23**, 1845 (*reaction*)
Kubow, S.A. *et al*, *Inorg. Chem.*, 1988, **27**, 2761 (*reaction*)
Rillema, D.P. *et al*, *Inorg. Chem.*, 1990, **29**, 167 (*reaction*)

$C_{10}H_8Cl_4N_2Tc$ IC-006737

(2,2′-Bipyridine-*N,N′*)tetrachlorotechnetium

Tetrachloro(2,2′-bipyridyl)technetium(IV). *2,2′-Bipyridyltechnetium tetrachloride*



M 396.9

Octahedral. Synth. from $TcCl_4$ and bipy via $[Tc(bipy)_2Cl_2]Cl_2$. Red-brown solid. Sol. DMF (with dec.).

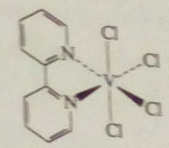
Fergusson, J.E. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 2293 (*synth, uv, magnetism*)

$C_{10}H_8Cl_4N_2V$ IC-006738

(2,2′-Bipyridine-*N,N′*)tetrachlorovanadium(*IV*), 9Cl

Tetrachloro(bipyridyl)vanadium(IV)

[30673-82-6]



M 348.9

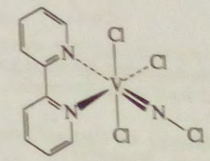
Octahedral. Synth. by distilling VCl_4 into a soln. of bipy in C_6H_6 or CCl_4. Brown solid; readily hydrol. to $VOCl_2$(bipy). Paramagnetic, $\mu_{eff} = 1.77\mu_B$ (300K), $1.60\mu_B$ (80K).

Clark, R.J.H., *J. Chem. Soc.*, 1963, 1377 (*synth, uv-vis, ir, magnetism*)

$C_{10}H_8Cl_4N_3V$ IC-006739

(2,2′-Bipyridine-*N,N′*)trichloro(chloroimido)vanadium(*V*), 10Cl

[71229-46-4]



M 362.9

Octahedral complex. Synth. by adding bipy to Cl_3VNCl in CH_2Cl_2 or CCl_4. Green-yellow solid. Sol. MeCN. A number of other adducts of Cl_3VNCl are known including those with $2SbCl_5$, 2Py, $2Ph_3P$. $\mu_{eff} = 0.55\mu_B$ (293K).

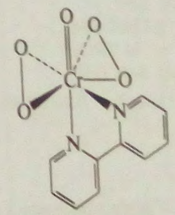
Loercher, K.P. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **452**, 123 (*synth, cryst struct, ir, magnetism*)

$C_{10}H_8CrN_2O_5$ IC-006740

(2,2′-Bipyridine-*N,N′*)oxodiperoxychromium(*VI*), 9Cl

(2,2′-Bipyridyl)oxodiperoxochromium(VI).
Oxidodi(peroxido)-2,2′-bipyridylchromium(VI)

[20911-38-0]



M 288.1

Pentagonal bipyramidal. Oxidant for org. synth. Blue solid. Spar. sol. CH_2Cl_2, $CHCl_3$, C_5H_5, Me_2CO. Mp 153° dec. Relat. compd. is Oxodiperoxy(pyridine) chromium(*VI*), IC-004695. Phenanthroline analogue also known.

Stomberg, R. *et al*, *Acta Chem. Scand.*, 1968, **22**, 1439 (*cryst struct*)
Firouzabadi, H. *et al*, *Tetrahedron*, 1986, **42**, 719 (*use*)

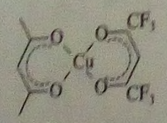
IC-006741

$C_{10}H_8CuF_6O_4$

(1,1,1,5,5,5-Hexafluoro-2,4-pentanedionato-O,O')(2,4-pentanedionato-O,O')copper(*II*), 11CI

(Acetylacetonato)(hexafluoroacetylacetonato)copper(II)

[21429-77-6]



M 369.7

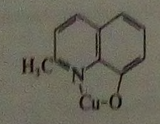
Approx. sq. planar coordination; Cu—O_{av} 194.6 pm. Green cryst.

Stabnikov, P.A. *et al*, *Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk*, 1982, 75 (*props*)
Baidina, I.A. *et al*, *Koord. Khim.*, 1984, **10**, 1699 (*cryst struct*)
Le Brun, P.C. *et al*, *Inorg. Chem.*, 1986, **25**, 3106 (*cryst struct*)

IC-006742

$C_{10}H_8CuNO$

(2-Methylquinolin-8-olato-N^1,O^8)copper(*I*)



M 221.7

Not obtd. without supporting ligands (e.g. CO); reaction of CuCl with L leads to Cu(*II*) complex. Binds CO, RNC, R_3P etc.

CO complex (tetrameric): see *Carbonyl(2-methyl-8-quinolinolato)copper*, *IC-007273*

p-Tolyl isocyanide complex: [87800-12-2]. *(1-Isocyano-4-methylbenzene)(2-methyl-8-quinolinolato-N^1,O^8)copper*
$C_{18}H_{16}CuN_2O$ M 338.8
Yellow cryst. Sol. THF. Tetrameric struct. proposed analogous to that of the CO complex. Ir $\nu_{C\equiv N}$ 2145 cm^{-1} (nujol).

Dppm complex (2:1): [115685-62-6]. *[μ-Methylenebis[diphenylphosphine]-P,P'][bis[μ-(8-quinolinolato-N^1,O^8:O^8)]dicopper*
$C_{49}H_{38}Cu_2N_2O_2P_2$ M 827.8
Yellow cryst. Sol. THF.

Dppe complex (1:1): [115669-37-9]. *[1,2-Ethanediylbis[diphenylphosphine]-P,P'](2-methyl-8-quinolinolato-N^1,O^8)copper*
$C_{36}H_{32}CuNOP_2$ M 620.1
Yellow cryst. Sol. THF.

Bis-PPh_3 complex: [115669-38-0].
$C_{46}H_{38}CuNOP_2$ M 746.3
Light yellow cryst. Sol. THF.

Floriani, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1988, 1607 (*synth, cryst struct, ir*)

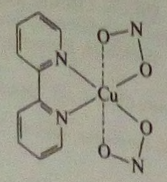
IC-006743

$C_{10}H_8CuN_4O_4$

(2,2'-Bipyridine-N,N')bis(nitrito)copper(*II*)

Bis(nitrito)-2,2'-bipyridylcopper(II)

[39771-80-7]



M 311.7

Pseudo-square planar. Cryst. Insol. EtOH.

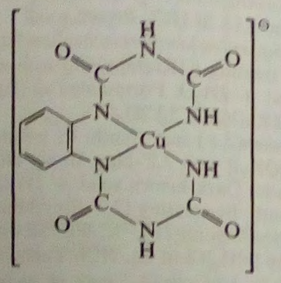
Stephens, F.S. *et al*, *J. Chem. Soc. A*, 1969, 2081 (*cryst struct*)
Procter, I.M. *et al*, *J. Inorg. Nucl. Chem.*, 1972, **34**, 3689 (*synth, ir, esr, uv*)

IC-006744

$C_{10}H_8CuN_6O_4^{\ominus}$

[N,N'''-1,2-Phenylenebis[imidodicarbonic diamidato]-N,N',N'',N''']cuprate(*III*)(1−), 10CI

o-Phenylenebis(biuretato)cuprate(III)



M 339.7 (ion)

Square planar.

Tetrabutylammonium salt: [63665-56-5].
Dark green needles. Sol. DMSO; insol. $CHCl_3$.

Birker, P.J.M.W.L., *Inorg. Chem.*, 1977, **16**, 2478 (*synth, cryst struct, pmr, electrochem*)
Birker, P.J.M.W.L., *J. Chem. Soc., Chem. Commun.*, 1977, 445 (*cryst struct*)
Brown, D.G. *et al*, *Inorg. Chem.*, 1980, **19**, 264 (*pe*)

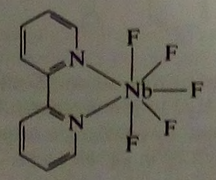
IC-006745

$C_{10}H_8F_5N_2Nb$

(2,2'-Bipyridine-N,N')pentafluoroniobium(*V*), 11CI

(α,α'-*Bipyridyl*)*pentafluoroniobium*(V)

[30233-11-5]



M 344.0

7-Coordinate. Synth. by reaction of NbF_5 and excess bipy in C_6H_6, toluene or MeCN. Pale yellow v. moisture-sensitive solid. Mp 172° dec.

Djordjevic, C. *et al*, *J. Chem. Soc. A*, 1970, 3382 (*synth, ir*)
Ignatov, M.E. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 345 (*synth, ir*)

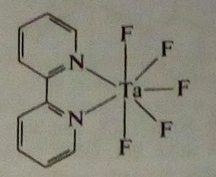
IC-006746

$C_{10}H_8F_5N_2Ta$

(2,2'-Bipyridine-N,N')pentafluorotantalum(*V*), 11CI

(α,α'-*Bipyridyl*)*pentafluorotantalum*(V). *Tantalum*(V) *fluoride 2,2'-bipyridine*

[85585-12-2]



M 432.1

7-Coordinate, detailed geometry unknown. Synth. from bipy and TaF_5(tributylphosphate) in toluene or MeCN. White solid.

Ignatov, M.E. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 617 (*synth, ir*)

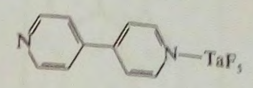
IC-006747

$C_{10}H_8F_5N_2Ta$

(4,4'-Bipyridine-N)pentafluorotantalum(*V*), 11CI

(γ,γ'-*Bipyridyl*)*pentafluorotantalum*(V). *Tantalum*(V) *fluoride γ,γ'-bipyridine*

[85585-13-3]



M 432.1

Octahedral. Synth. from TaF_5(tributylphosphate) and 4,4'-bipy in toluene or MeCN. White solid. If a 2:1 ratio of TaF_5 to ligand is used a dimer, F_5Ta-bipy-TaF_5 is formed.

Ignatov, M.E. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 617 (*synth, ir*)

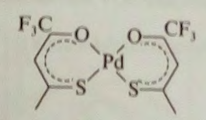
IC-006748

$C_{10}H_8F_6O_2PdS_2$

Bis(1,1,1-trifluoro-4-thioxo-2-pentanonato-O,S)palladium, 9CI

Bis(1,1,1-trifluoropentane-4-thione-2-onato)palladium(II)

[15744-67-9]



M 444.7

Square planar; precise stereochem. not reported. Synth. from K_2PdCl_4 and ligand. Orange cryst. (aq. Me_2CO). Mp 157-158°.

[55029-41-9]

Ho, R.K.Y. *et al*, *Aust. J. Chem.*, 1966, **19**, 1179 (*synth*)
Siimann, O. *et al*, *J. Chem. Phys.*, 1971, **54**, 740 (*ir*)
Das, M. *et al*, *Aust. J. Chem.*, 1974, **27**, 749 (*ms*)

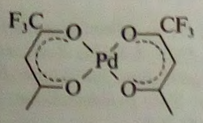
IC-006749

$C_{10}H_8F_6O_4Pd$

Bis(1,1,1-trifluoropentane-2,4-dionato-O,O')palladium(*II*), 10CI

Palladium trifluoroacetylacetonate

[63742-52-9]



M 412.5

Only known in *cis*- square planar form. Many studies of complex formation with mono- and bidentate ligands.

cis-form [65337-68-0]
Orange-yellow needles (CH_2Cl_2/hexane). Sol. C_6H_6, $CHCl_3$.

trans-form [77984-03-3]
Existence not confirmed.

Das, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 1409 (*dipole moment*)
Okeya, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 1085 (*synth, pmr, cmr, ir, F-19 nmr*)

Das, M. *et al*, *Inorg. Chim. Acta*, 1983, **76**, L111 (*ms*)
Baidina, I.A. *et al*, *Koord. Khim.*, 1986, **12**, 404 (*cryst struct*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **2**, 389 (*reactions*)

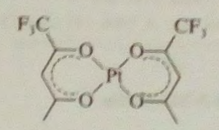
IC-006750

$C_{10}H_8F_6O_4Pt$

Bis(1,1,1-trifluoropentane-2,4-dionato-O,O')platinum, 10CI

Bis(trifluoroacetylacetonato)platinum(II)

[63742-53-0]



cis-form

M 501.2

Isomers resist interconversion. Ligand known as tfac.

cis-form [67596-99-0]
Yellow needles. Sol. many org. solvs. Subl. 108-111°.

trans-form [76740-70-0]
Yellow needles. Sol. many org. solvs.

Inorg. Synth., 1980, **20**, 65 (*synth*)
Okeya, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 1085 (*ir, pmr, cmr, F-19 nmr*)

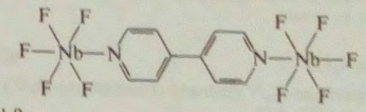
IC-006751

$C_{10}H_8F_{10}N_2Nb_2$

[μ-(4,4'-Bipyridine-$N:N'$)]decafluorodiniobium(*V*), 11CI

[μ-(γ,γ'-*Bipyridyl*)]*decafluorodiniobium*(V)

[85585-16-6]



M 531.9

Octahedral dimer. Synth. from NbF_5 -tributyl phosphate complex and 4,4'-bipy in toluene or MeCN. Sol. DMSO.

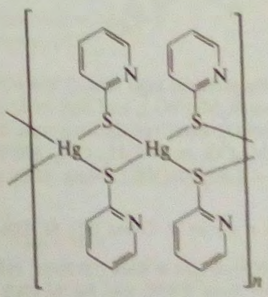
Ignatov, M.E. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1983, **28**, 345 (*synth, ir*)

IC-006752

$C_{10}H_8HgN_2S_2$

Bis(2-pyridinethionato)mercury

Mercury 2-pyridinethiolate



M 420.9

Square planar Hg in polymeric chain struct. Colourless cryst. (CH_2Cl_2/Et_2O). Mp 191°.

Wang, S. *et al*, *Inorg. Chem.*, 1989, **28**, 2615 (*synth, pmr, cryst struct*)

IC-006753

$C_{10}H_8I_2N_3ORu$

(2,2′-Bipyridine-*N*,*N*′)diiodo(nitrosyl)ruthenium, 9CI

[15635-37-7]

$$[Ru(NO)I_2(bipy)]_n \ (n \geqslant 2)$$

M 541.0

Probably dimeric. Prepd. by treating Diiodo(nitrosyl) ruthenium, IC-020215 with bipy in C_6H_6. Air-stable brown solid. Ir ν_{NO} 1848, 1795 cm^{-1}.

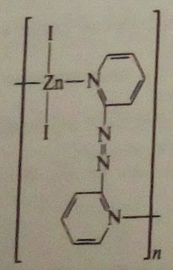
Irving, R.J. *et al*, *J. Chem. Soc. A*, 1966, 161 (*synth, ir*)

IC-006754

$C_{10}H_8I_2N_4Zn$

[2,2′-Azobis[pyridine]-*N*′]diiodozinc

[58080-46-9]



M 503.3

Polymeric in solid state. Solid.

Grzeskowiak, R. *et al*, *Spectrochim. Acta, Part A*, 1975, **31**, 1577 (*synth, ir, raman*)

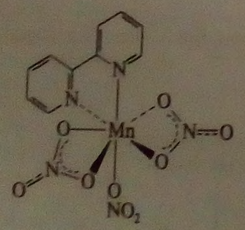
IC-006755

$C_{10}H_8MnN_2O_5$

(2,2′-Bipyridine-*N*,*N*′)(nitrato-*O*)bis(nitrato-*O*,*O*′) manganese(*III*), 9CI

2,2′-Bipyridyltris(nitrato)manganese(III)

[40905-56-4]



M 397.1

Pentagonal bipyramidal high spin d^4 Mn(*III*) complex. Synth. from $K_2Mn(NO_3)_4$ and bipy or $Mn(NO_3)_3$ and bipy in $MeNO_2$. Dark red dichroic cryst. Sol. MeCN; spar. sol. Me_2CO; insol. C_6H_6, CCl_4, $MeNO_2$; dec. by H_2O. μ_{eff} = 5.0μ_B (295K). Corresp. phen complex also known.

Johnson, D.W. *et al*, *Can. J. Chem.*, 1972, **50**, 3326 (*synth, ir, uv, magnetism*)

Einstein, F.W.B. *et al*, *Can. J. Chem.*, 1972, **50**, 3332 (*cryst struct*)

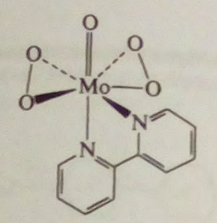
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 217 (*rev, bibl*)

$C_{10}H_8MoN_2O_5$ IC-006756

(2,2′-Bipyridine-*N*,*N*′)oxodiperoxymolybdenum(*VI*), 11CI, 10C, 9CI

Bipyridyloxodiperoxomolybdenum(VI)

[23319-62-2]



M 332.1

Distorted trigonal bipyramidal (or pentagonal bipyramidal) with asymmetrically bonded peroxo ligands; several analogous complexes also known. Oxidising agent. Yellow cryst. (DMF). Ir $\nu_{Mo=O}$ 940, ν_{O-O} 865 cm^{-1}.

Mimoun, H. *et al*, *Bull. Soc. Chim. Fr.*, 1969, **5**, 1481 (*synth, props*)

Schmitt, G. *et al*, *J. Organomet. Chem.*, 1976, **122**, 295 (*reactions*)

Winter, W. *et al*, *Inorg. Chem.*, 1980, **19**, 2045.

Schlemper, E.D. *et al*, *Polyhedron*, 1984, **3**, 377 (*cryst struct*)

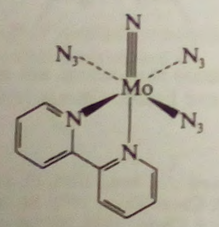
IC-006757

$C_{10}H_8MoN_{12}$

Triazido(2,2′-bipyridine-*N*,*N*′)nitridomolybdenum(*VI*), 10CI

Triazidonitridobipyridylmolybdenum(VI)

[75455-88-8]



M 392.1

Red cryst. Hydrol. easily. V. sol. 1,2-dichloroethane.

▷ Explosive.

Schweda, E. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1146 (*cryst struct, synth*)

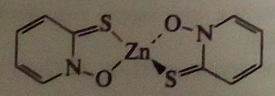
IC-006758

$C_{10}H_8N_2O_2S_2Zn$

Bis[1-hydroxy-2(1*H*)-pyridinethionato-*O*,*S*]zinc, 11CI

***Pyrithione zinc*, INN, USAN.** *Zinc polyanemine. Omadine OM 1563. Zinc pyrithione. Bis(2-pyridylthio) zinc 1,1′-dioxide. Zinc pyridinethione. Zinc omadine. Desquaman. Vancide ZP*

[13463-41-7]



M 317.7

Antibacterial, antifungal, antiseborrheic agent. Formerly used commercially as a pesticide. White solid. Sol. DMSO, DMF, $CHCl_3$. Mp 262°.

▷ ZH0950000.

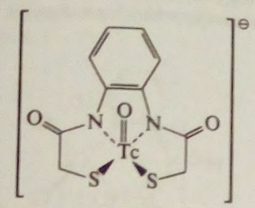
Robinson, M.A., *J. Inorg. Nucl. Chem.*, 1964, **26**, 1277 (*synth, ir*)

Martindale, The Extra Pharmacopoeia, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, **28/29**, 1633.

Steinbrech, B. *et al*, *Fresenius' Z. Anal. Chem.*, 1983, **316**, 465 (*synth, uv*)

$C_{10}H_8N_2O_3S_2Tc^{\ominus}$ IC-006759

Oxo[[*N*,*N*′-1,2-phenylenebis[2-mercaptoacetamidato]] (4−)-*N*,*N*′,*S*,*S*′]technetate(*V*)(1−), 10CI



M 367.2 (ion)

Synth. from $TcO_4^{\ominus}$ + H_4L with dithionite reduction.

Ph_4As salt: [75949-50-7].

Yellow-gold plates (EtOH aq.). Mp 221-225° dec.

Davison, A. *et al*, *Inorg. Chem.*, 1981, **20**, 1629 (*synth, uv, ir, pmr*)

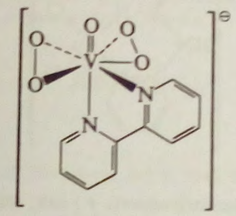
IC-006760

$C_{10}H_8N_2O_5V^{\ominus}$

(2,2′-Bipyridine-*N*,*N*′)oxodiperoxyvanadate(*V*)(1−), 11CI

(2,2′-Bipyridyl)oxobis(peroxo)vanadate(V)(1−)

[68832-77-9]



M 287.1 (ion)

Pentagonal bipyramidal, V displaced form plane by 32 pm towards O.

K salt: [42494-71-3].

Synth. from V_2O_5 in KOH, 20% H_2O_2 and bipy in EtOH. Yellow cryst. + $5H_2O$.

NH_4 salt: [88359-14-2].

Synth. from bipy in EtOH and a cooled soln. of NH_4VO_3 in 20% H_2O_2. Yellow cryst. + $4H_2O$.

Vuletic, N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1137 (*synth*)

Szentivanyi, H. *et al*, *Acta Chem. Scand., Ser. A*, 1983, **37**, 553 (*cryst struct, NH_4 salt*)

Schwendt, P., *Collect. Czech. Chem. Commun.*, 1983, **48**, 248 (*ir*)

Campbell, N.J. *et al*, *Inorg. Chim. Acta*, 1983, **77**, L215 (*cryst struct, NH_4 salt*)

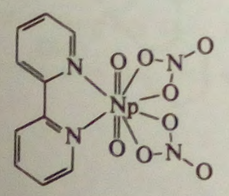
IC-006761

$C_{10}H_8N_4NpO_8$

(2,2′-Bipyridine-*N*,*N*′)bis(nitrato-*O*,*O*′)dioxoneptunium, 11CI

(Bipyridyl)dinitratodioxoneptunium(VI)

[90901-27-2]



M 549.2

8-Coordinate. Cryst. Similar acetate complex also prepd.

Alcock, N.W. *et al*, *Inorg. Chim. Acta*, 1984, **94**, 279.

Alcock, N.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 1001 (*synth, cryst struct*)

$C_{10}H_8N_4O_6Pt$

(2,2′-Bipyridine-*N*,*N*′)bis(nitrato)platinum, 9CI IC-006762

(2,2′-Bipyridyl)dinitratoplatinum(II)

[54822-51-4]

As (2,2′-Bipyridine-*N*,*N*′)dichloroplatinum, IC-006724 with

$$X = -ONO_2$$

M 475.2

Synth. from $Pt(bipy)(OH)_2$ + HNO_3. Orange-yellow solid. Sol. H_2O.

Bielli, E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2133.

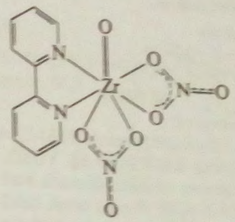
IC-006763

$C_{10}H_8N_4O_7Zr$

(2,2′-Bipyridine-*N*,*N*′)bis(nitrato-*O*,*O*′)oxozirconium(*IV*), 11CI

(α,α′-Bipyridyl)bis(nitrato)oxozirconium(IV)

[84821-78-3]



M 387.4

7-coordinate but geometry not reported. Synth. from $ZrO(NO_3)_2$ and ligand in MeOH. Moisture-stable solid. Sol. $PhNO_2$.

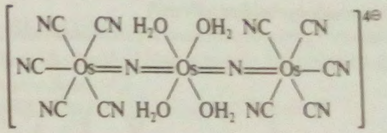
Srivastava, A.K. *et al*, *Croat. Chim. Acta*, 1982, **55**, 429; *CA*, **98**, 190543y (*synth, ir*)

IC-006764

$C_{10}H_8N_{12}O_4Os_3^{4\ominus}$

Tetraaquadecakis(cyano-*C*)di-μ-nitridotriosmate(*IV*) (4−), 11CI

μ-[Tetraaquabisnitridoosmium(IV)] *bis[pentacyanoosmate*(IV)]



M 930.8 (ion)

Tetra-K salt: [76247-74-0].

Hall, J.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 2410.

Griffith, W.P. *et al*, *Inorg. Chim. Acta*, 1987, **126**, 179 (*ir, cmr*)

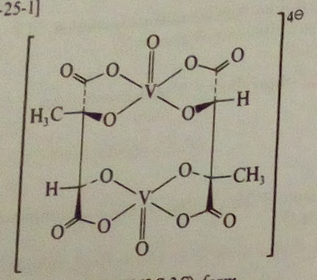
IC-006765

$C_{10}H_8O_{14}V_2^{4\ominus}$

Bis[μ-(2-methyltartrato)]dioxodivanadate(*IV*)(4−)

Bis[μ-[2,3-dihydroxy-2-methylbutanedioato(4−)-O^1,O^2:O^3,O^4]]dioxodivanadate(IV)(4−), *11CI*. *(μ-(+)threo-Monomethyltartrato)(μ-(−)threo-monomethyltartrato) bis[oxovanadate*(IV)]

[63511-25-1]



(2R,3R)(2S,3S)-form

M 454.0 (ion)

Square pyramidal dimer. The various isomers may be obtained by using the appropriate (+) or (−) form of the acid. Similar compds. are formed with tartaric acid and dimethyl tartaric acid. The dimers show very weak magnetic interactions.

(2R,3R)(2S,3S)-form

D,L-form. *(+)(−)-form*

Tetra-Na salt: [79813-77-7].

$C_{10}H_8Na_4O_{14}V_2$ M 546.0

No synth. reported.

Tetra-Na salt, tetradecahydrate: [79854-25-4].

Synth. by adding $Ba(OH)_2$ to aq. $VOSO_4$ and the appropriate isomer of methyltartaric acid then adjusting to pH 11 with NaOH. Brown cryst. solid (60% EtOH aq.). A decahydrate and a dodecahydrate are known.

(2S,3S),(2S,3S)-form

L,L-form. *(−)(−)-form*

Na salts v. difficult to isol.: extremely water sol. Solid glasses analysing as octahydrates obt.

[63511-29-5, 63527-69-5, 63527-70-8, 63527-71-9, 63527-74-2]

Crawford, Van.H. *et al*, *J. Mol. Struct.*, 1977, **38**, 141 (*magnetism, esr*)

Hahs, S.K. *et al*, *Inorg. Chem.*, 1982, **21**, 664 (*synth, esr, ir, uv-vis, pKa, isom*)

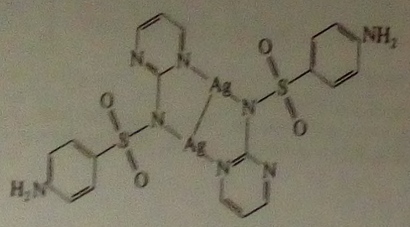
Ortega, R.B. *et al*, *Inorg. Chem.*, 1982, **21**, 672 (*cryst struct*)

$C_{10}H_9AgN_4O_2S$ IC-006766

(Sulfanilamidopyrimidine)silver(*I*)

(4-Amino-N-2-pyrimidinylbenzenesulfonamidato)silver, 9CI

[57533-85-4]



core dimer

M 357.1

Dimeric units are linked into chains by bridging pyrimidine N's and leading to overall trigonal bipyramidal coord. at Ag.

Dimer:

$C_{20}H_{18}Ag_2N_8O_4S_2$ M 714.2

Colourless cryst. Dec. in DMSO. Insol. EtOH.

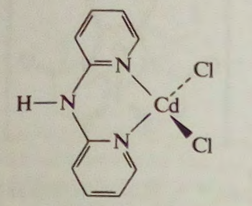
Baenziger, N.C. *et al*, *Inorg. Chem.*, 1976, **15**, 1807 (*cryst struct, synth*)

$C_{10}H_9CdCl_2N_3$ IC-006767

Dichloro(2,2′-dipyridylamine)cadmium(*II*)

Dichloro(2,2′-iminobispyridine)cadmium(II)

[18116-17-1]



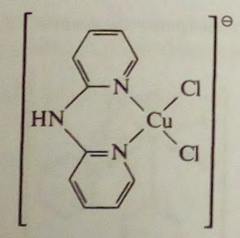
M 354.5

White solid (DMF/EtOH).

Black, D.St.C. *et al*, *Aust. J. Chem.*, 1967, **20**, 2101 (*synth*)

$C_{10}H_9Cl_2CuN_3^{\ominus}$ IC-006768

Dichloro[bis(2-pyridinyl)amine]cuprate(1−)



M 305.6 (ion)

Bis[di(2-pyridyl)amine]copper(1+) salt: see *Bis[di(2-pyridyl) amine]copper*(I)(*1+*), *IC-010439*

Bowmaker, G.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1989, 1639 (*synth, cryst struct, ir*)

$C_{10}H_9Co_2O_{10}P$ IC-006769

Heptacarbonyl(trimethyl phosphite)dicobalt

$(OC)_4Co{-}Co(CO)_3P(OMe)_3$

M 438.0

Ir ν_{CO} 2085.5, 2033, 2018, 1999.5, 1977 cm^{-1} (hexane).

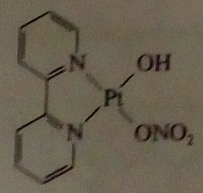
Szabo, P. *et al*, *J. Organomet. Chem.*, 1968, **12**, 245 (*synth, ir*)

$C_{10}H_9N_3O_4Pt$ IC-006770

(2,2′-Bipyridine-*N*,*N*′)hydroxy(nitrato-*O*)platinum(*II*), 9CI

2,2′-Bipyridyl(hydroxo)nitratoplatinum(II)

[54822-54-7]



M 430.2

Probably square planar structure with monodentate $NO_3^{\ominus}$, as shown. Synth. from $Pt(OH)_2(bipy)_2 + HNO_3$. Orange-yellow solid.

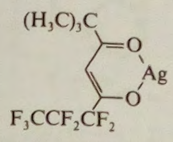
Bielli, E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 2133 (*synth*)

$C_{10}H_{10}AgF_7O_2$ IC-006771

(6,6,7,7,8,8,8-Heptafluoro-2,2-dimethyl-3,5-octanedionato-*O*,*O*′)silver, 11CI, 10CI, 9CI

(1,1,1,2,2,3,3-Heptafluoro-7,7-dimethyl-4,6-octanedionato) silver(I). *Ag(fod)*

[76121-99-8]



M 403.0

Nmr shift reagent; used in conjunction with $Yb(fod)_3$ and $Pr(fod)_3$ for aromatic protons. Light sensitive. Dec. on crystallisation. Insol. H_2O. Mp 134° dec.

Wenzel, T.J. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 5903 (*synth, use*)
Wenzel, T.J. *et al*, *Anal. Chem.*, 1981, **53**, 343 (*synth, use*)
Rackham, D.M. *et al*, *Spectrosc. Lett.*, 1981, **14**, 379, 639.
Audit, M. *et al*, *Org. Magn. Reson.*, 1983, **21**, 698 (*nmr studies*)
Hajek, M. *et al*, *Anal. Chem.*, 1986, **58**, 1743 (*use*)

$C_{10}H_{10}AsF_{15}O_5$ IC-006772

Pentakis(2,2,2-trifluoroethoxy)arsorane, 11CI

Pentakis(2,2,2-trifluoroethoxy)arsenic(V)

[96991-75-2]

$As(OCH_2CF_3)_5$

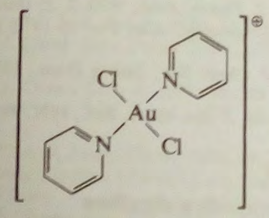
M 570.0

Liq. $Bp_{0.1}$ 54°.

Denney, D.B. *et al*, *Phosphorus Sulfur*, 1985, **22**, 33 (*synth, pmr, cmr, F-19 nmr*)

$C_{10}H_{10}AuCl_2N_2^{\oplus}$ IC-006773

Dichlorobis(pyridine)gold(*III*)(1+)



M 426.0 (ion)

Geometry intermediate between *trans*-sq. planar and tetrahedral. Cryst. as hydrate.

Chloride: [15679-82-0]. *Gold*(III) *chloride bis(pyridine)*

Dichloroaurate(1−) salt: [82025-08-9].

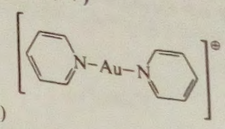
$C_{10}H_{10}Au_2Cl_4N_2$ M 693.9

[80339-11-3, 82025-31-8]

Jones, P.G., *Gold Bull.*, 1981, **14**, 102 (*rev*)
McConnell, A.A. *et al*, *Spectrochim. Acta, Part A*, 1981, **37**, 583 (*ir, raman*)
Adams, H.-N. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **485**, 65 (*synth, cryst struct*)
Chen, H.W. *et al*, *Inorg. Chim. Acta*, 1985, **96**, 137 (*synth*)

$C_{10}H_{10}AuN_2^{\oplus}$

Bis(pyridine)gold(*I*)(1+) IC-006774



M 355.1 (ion)

Dichloroaurate(1−): [22355-16-4]. *Chloro(pyridine)gold*(I)

$C_{10}H_{10}Au_2Cl_2N_2$ M 623.0

Light- and heat-sensitive colourless cryst.

Dibromoaurate(1−): [92361-26-7]. *Bromo(pyridine)gold*(I)

$C_{10}H_{10}Au_2Br_2N_2$ M 711.9

Light-sensitive triclinic or monoclinic cryst.

Diiodoaurate(1−): [82025-10-3]. *Iodo(pyridine)gold*(I)

$C_{10}H_{10}Au_2I_2N_2$ M 805.9

Light-sensitive colourless solid, dec. above −30°.

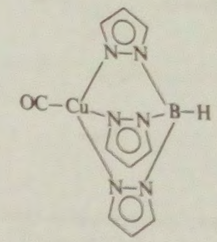
[82025-09-0]

Adams, H.N. *et al*, *Abstr. Eur. Cryst. Meeting*, 1977, 200 (*cryst struct*)
Jones, P.G. *et al*, *Gold Bull.*, 1981, **14**, 102 (*rev*)
Adams, H.N. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **485**, 81 (*synth, ir, cryst struct*)
Conzelmann, W. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **512**, 169 (*synth*)
Mirabell, C.K. *et al*, *J. Med. Chem.*, 1986, **29**, 218 (*tox, pharmacol*)

$C_{10}H_{10}BCuN_6O$ IC-006775

Carbonyl[hydrotris(1*H*-pyrazolato-N^1)borato(1−)-N^2,$N^{2'}$,$N^{2''}$]copper, 9CI

[52374-64-8]



M 304.5

Cryst. (pet. ether). Sol. Me_2CO, THF. Mp 164-166°. Stable under CO atm. Rapid oxid. in soln.

Bruce, M.I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2433 (*synth*)
Churchill, M.R. *et al*, *Inorg. Chem.*, 1975, **14**, 2051 (*cryst struct*)
Inorg. Synth., 1982, **21**, 108 (*synth*)

$C_{10}H_{10}BI_2N_6ORh$ IC-006776

Carbonyl[hydrotris(1*H*-pyrazolato-N^2)borato(1−)] diiodorhodium, 9CI

Carbonyldiiodo[tris(pyrazolyl)borato]rhodium

[52504-76-4]

M 597.7

Deep-red cryst. (CH_2Cl_2/hexane). Ir ν_{CO} 2095 cm^{-1} (KBr).

Cocivera, M. *et al*, *Organometallics*, 1982, **1**, 1125 (*synth, pmr, ir, struct*)

IC-006777

$C_{10}H_{10}Br_2CdN_2$

Dibromobis(pyridine)cadmium

Bis(pyridine)cadmium dibromide. Cadmium(II) *bromide bis(pyridine)*

[14872-07-2]

$[CdBr_2Py_2]_n$

M 430.4

Halide-bridged chain polymer with 6-coordinate Cd. Needles. Loses first Py at 120-190°; and second Py at 190-310°.

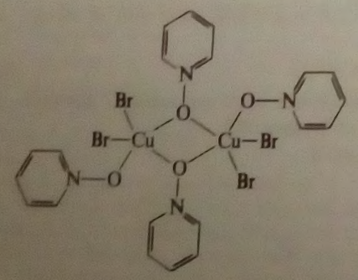
[39529-63-0]

Malinovskii, T.I. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1962, **147**, 96 (*cryst struct*)
Wendlandt, W.W. *et al, Z. Anorg. Allg. Chem.*, 1965, **337**, 6 (*thermal anal*)
Allan, J.R. *et al, J. Chem. Soc. A*, 1966, 1031 (*synth*)
Goldstein, M. *et al, J. Mol. Struct.*, 1972, **14**, 451 (*ir, raman*)
Babushkina, T.A. *et al, Koord. Khim.*, 1975, **1**, 1266 (*nqr*)
Akyuz, S. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1746 (*ir, raman*)

IC-006778

$C_{10}H_{10}Br_2CuN_2O_2$

Dibromobis(pyridine *N*-oxide)copper(*II*)



dimer

M 413.5

Dimeric.

Dimer: [28491-16-9]. *Tetrabromobis[μ-(pyridine 1-oxide-O:O)]bis(pyridine 1-oxide-O)dicopper*(II), *9Cl*
$C_{20}H_{20}Br_4Cu_2N_4O_4$ M 827.1
Synth. from $CuBr_2$ + ligand in 1-butanol. Cryst. (1-butanol). $\mu_{eff} = 1.4\mu_B$.

Watson, W.H., *Inorg. Chem.*, 1969, **8**, 1879 (*synth*)
Mighell, A.D. *et al, Acta Crystallogr., Sect. B*, 1972, **28**, 126 (*cryst struct, magnetism*)

IC-006779

$C_{10}H_{10}Br_2HgN_2$

Dibromobis(pyridine)mercury(*II*)

Bis(pyridine)mercury dibromide. Mercury(II) *bromide bis(pyridine)*

[15632-04-9]

Py_2HgBr_2

M 518.6

Monomeric. Tetrahedral mercury both in the solid state and in soln. Cryst. (Py). Readily loses Py.

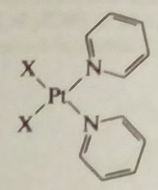
[28108-22-7]

Hieber, W. *et al, Z. Elektrochem.*, 1938, **44**, 881 (*synth*)
Clark, R.J.H. *et al, Chem. Ind. (London)*, 1964, 1317 (*ir*)
Ahuja, I.S. *et al, J. Chem. Soc. A*, 1970, 2161 (*synth, ir*)
Barr, R.M. *et al, J. Cryst. Mol. Struct.*, 1974, **4**, 165 (*ir, raman*)
Babushkina, T.A. *et al, Koord. Khim.*, 1975, **1**, 1266 (*nqr*)
Canty, A.J. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 15 (*cryst struct, struct*)
Persson, I. *et al, J. Chem. Soc., Dalton Trans.*, 1985, 1597 (*cryst struct, synth, ir, raman, soln struct*)

IC-006780

$C_{10}H_{10}Br_2N_2Pt$

Dibromobis(pyridine)platinum(*II*)



cis-form

X = Br

M 513.0

trans-form more easily prepared than *cis*.

cis-form [14049-74-2]

Phys. props. not reported.

trans-form [14024-87-4]

Gmelin Handbook Inorg. Chem., Syst. No. 68, 1957, D, 286 (*synth*)
Adams, D.M. *et al, J. Chem. Soc.*, 1964, 734 (*ir*)
Dung, J.R. *et al, Spectrochim. Acta, Part A*, 1967, **23**, 1121 (*ir*)
Thompson, L.K. *et al, Inorg. Chim. Acta*, 1980, **38**, 117 (*synth, ir*)

IC-006781

$C_{10}H_{10}Br_2N_2Zn$

Dibromobis(pyridine)zinc(*II*)

Bis(pyridine)zinc dibromide. Zinc(II) *bromide bis(pyridine)*

[14024-88-5]

$(Py)_2ZnBr_2$

M 383.4

Tetrahedral at Zn. White cryst. (EtOH). Mp 220-222°.

Varet, L., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1891, **112**, 622 (*synth*)
Hieber, W. *et al, Z. Anorg. Allg. Chem.*, 1931, **196**, 193 (*synth*)
Coates, G.E. *et al, J. Chem. Soc.*, 1964, 166 (*ir*)
Clark, R.J.H. *et al, Inorg. Chem.*, 1965, **4**, 350 (*ir*)
Ablov, A.V. *et al, Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 1243 (*synth, heat of formn*)
Liptay, G. *et al, J. Therm. Anal.*, 1970, **2**, 25 (*thermal anal*)
Saito, Y. *et al, Spectrochim. Acta, Part A*, 1972, **28**, 1459 (*ir, raman*)
Akyuz, S. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1746 (*ir, raman*)
Hsieh, Yu.-N. *et al, J. Am. Chem. Soc.*, 1977, **99**, 1384 (*N-14 nqr*)

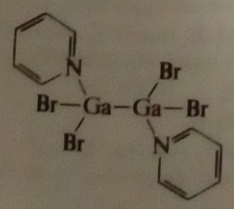
IC-006782

$C_{10}H_{10}Br_4Ga_2N_2$

Tetrabromobis(pyridine)digallium

Digallium tetrabromide bis(pyridine)

[80786-54-5]



M 617.2

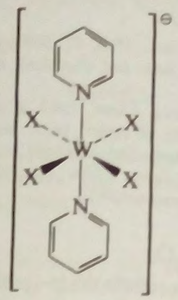
Synth. from Py and Ga_2Br_4 2(dioxan). White moisture-sensitive cryst. (Py). See also Gallium(*I*) tetrabromogallate(*III*), IC-002019.

Small, R.W.H. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 86 (*cryst struct*)

IC-006783

$C_{10}H_{10}Br_4N_2W^{\ominus}$

Tetrabromobis(pyridine)tungstate(*III*)(1−), 10Cl



X = Br

M 661.6 (ion)

Octahedral. W—Br_{av} 258, W—N_{av} 218 pm.

Pyridinium salt, pyridine compd.: [72664-37-0]. $Py_2H^{\oplus}$ *salt* Obt. from $WBr_4(Py)_2$ reduced by Py at 55° *in vacuo*. V. air- and moisture-sensitive cryst.

Brencic, J.V. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 3028 (*cryst struct*)

IC-006784

$C_{10}H_{10}CdCl_2N_2$

Dichlorobis(pyridine)cadmium

Bis(pyridine)cadmium dichloride. Cadmium(II) *chloride bis(pyridine)*

[14024-90-9]

$(Py)_2CdCl_2$

M 341.5

Has polymeric chain struct. with octahedral Cd and bridging chloride. White cryst. Loses Py on heating. Dissoc. in H_2O.

[25867-37-2, 39529-62-9]

Lang, W., *Chem. Ber.*, 1888, **21**, 1578.
Zannetti, R. *et al, Gazz. Chim. Ital.*, 1960, **90**, 1428 (*cryst struct*)
Nagano, K. *et al, Chem. Pharm. Bull.*, 1964, **12**, 1198 (*synth*)
Clark, R.J.H. *et al, Inorg. Chem.*, 1965, **4**, 350 (*ir*)
Wendlandt, W.W. *et al, Z. Anorg. Allg. Chem.*, 1965, **337**, 6 (*thermal dec*)
Goldstein, M. *et al, J. Mol. Struct.*, 1972, **14**, 451 (*ir, raman*)
Akyuz, S. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 1746 (*ir, raman*)
Basu, S., *Indian J. Chem., Sect. A*, 1978, **16**, 246 (*Cl-35 nqr*)
McConnell, A.A. *et al, J. Mol. Struct.*, 1978, **49**, 207 (*powder struct*)
Rubenackar, G.V. *et al, Inorg. Chem.*, 1980, **19**, 392 (*N-14 nqr*)
Han, X. *et al, Kexue Tongbao (Foreign Lang. Ed.)*, 1981, **26**, 1297; *CA*, **97**, 99814 (*cmr*)
Masuda, Y. *et al, Thermochim. Acta*, 1988, **128**, 225 (*thermal anal*)

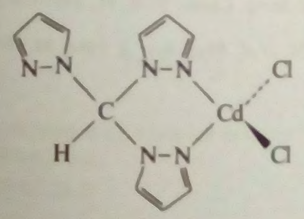
IC-006785

$C_{10}H_{10}CdCl_2N_6$

Dichloro[tris(1-pyrazolyl)methane]cadmium

Dichloro[1,1′,1″-methylidynetris[1H-pyrazole]-N^2,N^2] *cadmium*

[113873-04-4]



M 397.5

Tetrahedral Cd. Air- and moisture-stable colourless cryst. + $\frac{1}{2}H_2O$ (aq. EtOH). Sol. DMSO; insol. most other org. solvs. Mp 304-306°. Dissoc. in DMSO soln.

Lobbia, G.G. *et al, Synth. React. Inorg. Metal-Org. Chem.*, 1987, **17**, 909 (*synth, ir, pmr, cmr, conductivity*)

IC-006786

$C_{10}H_{10}CdI_2N_2$

Diiodobis(pyridine-*N*)cadmium(*II*), 9Cl

Bis(pyridine)cadmium diiodide. Cadmium(II) *iodide bis(pyridine)*

[14024-91-0]

$(Py)_2CdI_2$

M 524.4

Monomeric in solid state and in soln. Catalyst for acrolein polym. White cryst. Sol. C_5H_5N.

Hieber, W. *et al, Z. Elektrochem.*, 1940, **46**, 556 (*synth*)
Clark, R.J.H. *et al, Inorg. Chem.*, 1965, **4**, 350 (*ir, synth*)
Wendlandt, W.W. *et al, Z. Anorg. Allg. Chem.*, 1965, **337**, 6 (*thermal anal*)
Allan, J.R. *et al, J. Chem. Soc. A*, 1966, 1031 (*synth, ir*)
Goldstein, M. *et al, J. Mol. Struct.*, 1972, **14**, 451 (*ir, raman*)
Armstrong, R.S. *et al, J. Mol. Struct.*, 1975, **29**, 117 (*soln conform*)
Babushkina, T.A. *et al, Koord. Khim.*, 1975, **1**, 1266 (*nqr*)

IC-006787

$C_{10}H_{10}CdN_8$

Diazidobis(pyridine)cadmium

Bis(pyridine)cadmium diazide. Cadmium(II) *azide bis(pyridine)*

[31631-91-1]

$Cd(N_3)_2(Py)_2$

M 354.6

Octahedral Cd in solid state: 3-D framework with bridging azide units. Cryst. (Py).

[36516-05-9]

Curtius, T. *et al, J. Praki. Chem.*, 1898, **58**, 294.
Strecker, W. *et al, J. Praki. Chem.*, 1939, **152**, 215.
Agrell, I., *Acta Chem. Scand.*, 1970, **24**, 3575; 1971, **25**, 2965 (*synth, ir, cryst struct*)

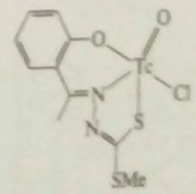
IC-006788

$C_{10}H_{10}ClN_2O_2S_2Tc$

Chloro[*S*-methyl-2-*N*-(2-hydroxyphenylethylidene) dithiocarbazato]oxotechnetium(*V*)

Chloro[methyl[1-(2-hydroxyphenyl)ethylidene] hydrazinecarbodithioato(2−)-N^2,O^2,S^3]*oxotechnetium, 12Cl*

[110485-56-8]



M 388.6

Tentative struct. shown. Synth. from $[TcOCl_4]^{\ominus}$. Paramagnetic golden-brown solid, or red cryst. (CH_2Cl_2/EtOH). Non-electrolyte. Insol. H_2O, alcohols; sol. Me_2CO, DMF, CH_2Cl_2, $CHCl_3$.

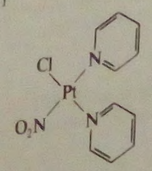
Du Preez, J.G.H. *et al, Inorg. Chim. Acta*, 1987, **130**, 9 (*synth, ir, uv, conductivity*)

$C_{10}H_{10}ClN_3O_2Pt$ IC-006789

Chloro(nitrito)bis(pyridine)platinum(*II*), 10Cl

Chloro(nitro)bis(pyridine)platinum(II), *8Cl*

[22668-79-7]



cis-form

M 434.7

Square planar.

cis-form [70812-17-8]

White solid. Sol. MeOH.

trans-form [70774-90-2]

White cryst. Sol. many org. solvs.

Kotowski, M. *et al*, *Inorg. Chem.*, 1979, **18**, 2555 (*kinetics*)

$C_{10}H_{10}Cl_2CoN_2$ IC-006790

Dichlorobis(pyridine)cobalt(*II*), 8Cl

Cobalt(II) *chloride bis(pyridine)*

$CoCl_2(Py)_2$

M 288.0

Prototype of many CoL_2X_2 compds. (L = pyridine or derivative, X = coordinating anion).

Monomeric-form [14024-92-1]

Tetrahedral struct. Obt. from polymeric form at 120° or by evaporation of $CHCl_3$ soln. Blue solid. Sol. $CHCl_3$, $MeNO_2$, $PhNO_2$.

Polymeric-form [26603-94-1]

Chain struct. with Cl-bridged octahedral CoN_2Cl_4 units. Synth. from $CoCl_2$ + Py. Formed from monomeric-form on standing in air. Violet solid. Sol. $CHCl_3$, $MeNO_2$, $PhNO_2$.

[29469-41-8]

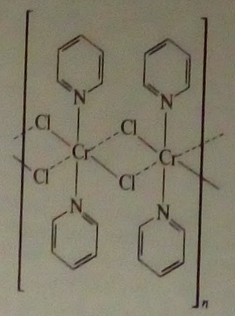
Gill, N.S. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **18**, 88 (*synth, uv*)
Clark, R.J.H. *et al*, *Inorg. Chem.*, 1965, **4**, 350 (*ir*)
Bentley, R.B. *et al*, *J. Chem. Soc. A*, 1971, 3751 (*magnetism*)
Clarke, P.J. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 1543 (*cryst struct*)

$C_{10}H_{10}Cl_2CrN_2$ IC-006791

Dichlorobis(pyridine)chromium(*II*), 10Cl, 9Cl

Chromium(II) *chloride bis(pyridine)*

[14320-05-9]



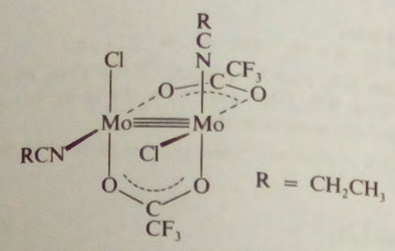
M 281.1

Chloride-bridged chain polymer; similar complexes of other halides and substituted pyridines also reported. Starting material. Light green air-sensitive solid. Antiferromagnetic.

Lux, H. *et al*, *Chem. Ber.*, 1964, **97**, 503 (*synth*)
Earnshaw, A. *et al*, *Chem. Ind. (London)*, 1965, 1521 (*synth, magnetism*)
Holah, D.G. *et al*, *Inorg. Chem.*, 1965, **4**, 1112.
Inorg. Synth., 1967, **10**, 26 (*synth, uv, ir, magnetism*)
Beech, G. *et al*, *J. Chem. Soc. A*, 1969, 512 (*tga*)
Khamar, M.M. *et al*, *Inorg. Chim. Acta*, 1978, **28**, 245; 1979, **36**, 223 (*synth, uv, ir, magnetism*)

$C_{10}H_{10}Cl_2F_6Mo_2N_2O_4$ IC-006792

Dichlorobis(propanenitrile)bis[μ-(trifluoroacetato-*O*:*O*′)]dimolybdenum(*II*), 11Cl



R = CH_2CH_3

M 598.9

Mo—Mo 212.7 pm. See note under Chloro(propanenitrile)tris[μ-(trifluoroacetato-*O*:*O*′)]dimolybdenum(*II*), IC-006460. Orange cryst.

[89659-47-2]

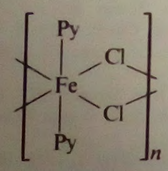
Agaskar, P. *et al*, *Inorg. Chim. Acta*, 1984, **83**, 33 (*synth, cryst struct*)

$C_{10}H_{10}Cl_2FeN_2$ IC-006793

Dichlorobis(pyridine)iron(*II*)

Iron(II) *chloride bis(pyridine)*

[15616-26-9]



M 284.9

Polymeric chain struct. with symmetrically bridging chlorides. Phase transition to asymmetric bridging at low temp. Synth. from $FeCl_2$ + Py in MeOH or by heating $Fe(Py)_4Cl_2$. Catalyst for peroxide dec. Synthetic intermediate. Golden yellow cryst. Rel. stable in dry air. Quasi-1D ferromagnet.

[27835-83-2]

Inorg. Synth., 1939, **1**, 184 (*synth*)
Long, G.J. *et al*, *Inorg. Chem.*, 1971, **10**, 1407 (*synth, mössbauer, magnetism, ir*)
Akyüz, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1746 (*ir*)
Little, B.F. *et al*, *Inorg. Chem.*, 1978, **17**, 3401 (*mössbauer, magnetism*)
De Groot, H.J.M. *et al*, *Phys. Rev. B*, 1984, **30**, 4041 (*mössbauer*)

$C_{10}H_{10}Cl_2HgN_2$ IC-006794

Dichlorobis(pyridine)mercury(*II*)

Bis(pyridine)mercury dichloride. Mercury(II) *chloride bis(pyridine)*

[15632-09-4]

Py_2HgCl_2

M 429.6

Polymeric in the solid state with octahedral Hg; monomeric (tetrahedral Hg) in soln. (C_{2v}). Cryst. (Py). Mp 106°. Readily loses Py.

[28108-21-6]

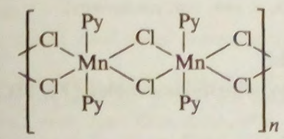
Hieber, W. *et al*, *Z. Elektrochem.*, 1938, **44**, 881 (*synth*)
Clark, R.J.H. *et al*, *Inorg. Chem.*, 1965, **4**, 350 (*ir*)
Ahuja, I.S. *et al*, *J. Chem. Soc. A*, 1970, 2161 (*synth, ir*)
Barr, R.M. *et al*, *J. Cryst. Mol. Struct.*, 1974, **4**, 165 (*ir, raman*)
Basu, *Indian J. Chem., Sect. A*, 1978, **16**, 245 (*nqr*)
Han, X. *et al*, *Kexue Tongbao (Foreign Lang. Ed.)*, 1981, **26**, 1297; *CA*, 1982, **96**, 134613 (*cmr*)
Canty, A.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 15 (*synth, cryst struct*)
Persson, I. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 1597 (*x-ray, synth, ir, raman, soln struct*)
Yang, Z. *et al*, *CA*, 1986, **104**, 13879 (*Hg-199 nmr*)

$C_{10}H_{10}Cl_2MnN_2$ IC-006795

Dichlorobis(pyridine)manganese(*II*), 11Cl

Manganese dichloride bispyridine. Manganese(II) *chloride bispyridine*

[14872-18-5]



M 284.0

Polymeric. Synth. from $MnCl_2$ and Py in EtOH. Pink needle-shaped cryst. Sol. H_2O, MeOH, insol. Et_2O, C_6H_6. $MnCl_2Py_2$ has been reported as stable in air but earlier work reported the compd. to be deliquescent. Antiferromagnetic at low temps. Analogous $MnBr_2$ Py_2 shows catalytic activity in oxidation of dodecylbenzene and 3,5 diethylbenzene.

Gill, N.S. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **18**, 79, 88 (*ir, synth*)
Goldstein, M. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 1107 (*far ir*)
Richards, P.M. *et al*, *J. Chem. Phys.*, 1973, **59**, 4474 (*cryst struct*)
Witteveen, H.T. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 1535 (*magnetism*)
Klaaijsen, F.W. *et al*, *Physica B+C (Amsterdam)*, 1976, **81**, 1 (*Cp*)
Hronec, M. *et al*, *Collect. Czech. Chem. Commun.*, 1980, **45**, 880 (*catalysis prop*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 92 (*rev, bibl*)

$C_{10}H_{10}Cl_2N_2Ni$ IC-006796

Dichlorobis(pyridine)nickel(*II*), 9Cl

Nickel(II) *chloride bis(pyridine)*

[32104-38-4]

$[NiPy_2Cl_2]_n$

M 287.7

Octahedral polymer with chlorine bridges. Yellow-green solid. Paramagnetic.

[14024-96-5, 26602-22-2]

Gill, N.S. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **18**, 88 (*synth, uv, magnetism*)
Goodgame, D.M.L. *et al*, *J. Chem. Soc.*, 1964, 5194; *J. Chem. Soc. A*, 1966, 1769 (*uv*)
Rowley, D.A. *et al*, *Inorg. Chem.*, 1968, **7**, 795 (*uv*)
McConnell, A.A. *et al*, *J. Mol. Struct.*, 1978, **49**, 207 (*polymer, powder struct*)

$C_{10}H_{10}Cl_2N_2OV$ IC-006797

Dichlorooxobis(pyridine)vanadium(*IV*), 10Cl

[68510-49-6]

$VOCl_2(Py)_2$

M 296.0

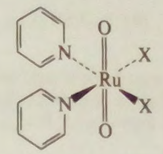
Probably square pyramidal. Synth. from $VOCl_2(MeCN)_2$ and Py in THF or MeCN, or from $VOCl_3.3MeOH$ + Py in Et_2O. Turquoise-blue solid. Paramagnetic, $\mu_{eff} \simeq 1.72\mu_B$.

Fowles, G.W.A. *et al*, *Inorg. Chim. Acta*, 1973, **7**, 642 (*synth, magnetism*)
Cave, J. *et al*, *Inorg. Chim. Acta*, 1978, **30**, L349 (*synth, ir*)

$C_{10}H_{10}Cl_2N_2O_2Ru$ IC-006798

Dichlorodioxobis(pyridine)ruthenium(*VI*), 9Cl

[122212-06-0]



X = Cl

M 362.1

Octahedral. Prepd. by treating RuO_4 in CCl_4 with mildly basic [PyH]Cl at 0°. Yellow diamagnetic complex. Ir ν_{RuO_2} 825 cm^{-1}.

[38856-18-7]

Griffith, W.P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir*)
El-Hendawy, A.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1989, 901 (*synth, use*)

$C_{10}H_{10}Cl_2N_2Pd$ IC-006799

Dichlorobis(pyridine)palladium(*II*), 9Cl, 8Cl

Palladium(II) *chloride bis(pyridine)*

$PdCl_2(Py)_2$

M 335.5

Both square planar isomers known; *trans*-form more stable. Many reports of carbonylation catalysis, often with other metal complexes. Possible use as photographic emulsion stabiliser.

cis-form [15227-47-1]

Synth. from H_2PdCl_6 or $Pd(PhSCH_2CH_2SPh)Cl_2$ + Py. Red needles. At 100° converts to *trans*-form.

trans-form [14052-12-1]

Synth. from H_2PdCl_6 + Py or from *cis*-form at 100°. Bright green solid.

Krauss, F. *et al*, *Z. Anorg. Allg. Chem.*, 1927, **165**, 73 (*synth*)
Cattalini, L. *et al*, *Gazz. Chim. Ital.*, 1968, **98**, 831 (*synth, ir*)
Pfeffer, M. *et al*, *Spectrochim. Acta, Part A*, 1974, **30**, 331 (*ir, raman*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **6**, 98, 290 (*use*)

IC-006800

$C_{10}H_{10}Cl_2N_2Pt$
Dichlorobis(pyridine)platinum(*II*), 8Cl
Platinum(II) *chloride bis-pyridine*
[14872-21-0]

As Dibromobis(pyridine)platinum(*II*), IC-006780 with

X = Cl

M 424.1
Square planar. Extensive studies on synth., struct., props. and reactions of both isomers.

cis-form [15227-42-6]
Sulfur yellow solid. Sol. $CHCl_3$, Me_2CO, DMF. Mp 224° dec.
▷ TP2498400.

trans-form [14024-97-6]
Pale yellow solid. Sol. C_6H_6, $CHCl_3$, Me_2CO, DMF. Mp 256° dec. More sol. than *cis*-isomer.
▷ TP2498500.

Inorg. Synth., 1963, **7**, 249 (*synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 429, 430, 495.

IC-006801

$C_{10}H_{10}Cl_2N_2RuS_2$
Dichlorobis(pyridine-2-thiol)ruthenium(*II*), 8Cl
[31390-34-8]

$[Ru(Py\text{-}2\text{-}SH)_2Cl_2]_n$

M 394.3
Struct. unknown; must be polymeric or oligomeric. Prepd. by treating methanolic Ruthenium blue, IC-017522 with pyridine-2-thiol. Brown solid. Ir ν_{RuCl} 306 cm^{-1} (vaseline).

Gilbert, J.D. *et al*, *J. Chem. Soc. A*, 1970, 2765 (*synth, ir*)

IC-006802

$C_{10}H_{10}Cl_2N_2Zn$
Dichlorobis(pyridine)zinc
[6843-20-5]

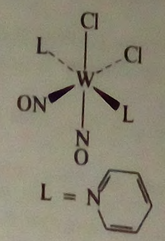
$ZnCl_2Py_2$

M 294.4
Prepd. from $ZnCl_2$ + Py. White needles (EtOH or Py). Mp 204-206°.

Long, W., *Ber.*, 1888, **21**, 1578 (*synth*)
Issopoulos, P.B., *Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **278**, 263 (*synth*)
Steffen, W.L. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 298 (*cryst struct*)
Akyuz, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 1746 (*ir, raman*)
Hutton, A.T. *et al*, *Spectrochim. Acta, Part A*, 1978, **34**, 645 (*ir*)

IC-006803

$C_{10}H_{10}Cl_2N_4O_2W$
Dichlorodinitrosylbis(pyridine)tungsten, 11Cl, 8Cl
[21338-23-8]



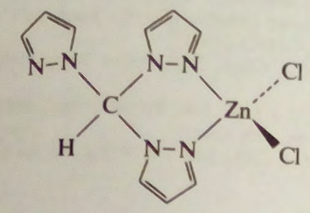
M 472.9
Octahedral, *cis*-dinitrosyl. Synth. from $W(NO)_2Cl_2$ + Py or by reductive nitrosylation of Na_2WO_4 by $NH_2OH.HCl$ in Py. For L = PPh_3, see Dichlorodinitrosylbis(triphenylphosphine)tungsten, IC-013180, L = $AsPh_3$, see Dichlorodinitrosylbis(triphenylarsine)tungsten, IC-013078.

[99603-52-8]

Cotton, F.A. *et al*, *Inorg. Chem.*, 1964, **3**, 1609 (*ir*)
Miyokawa, K. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 2791 (*gc*)
Sarkar, S. *et al*, *Chem. Lett.*, 1985, 1633 (*synth*)

IC-006804

$C_{10}H_{10}Cl_2N_6Zn$
Dichloro[tris(1-pyrazolyl)methane]zinc
Dichloro[*1,1′,1″-methylidynetris*[*1H-pyrazole*]-$N^2,N^{2'}$]*zinc*(II), *12Cl*
[113873-03-3]



M 350.5
Air- and moisture-stable colourless cryst. Sol. DMSO; sl. sol. EtOH, MeOH; insol. C_6H_6, CCl_4, $CHCl_3$, CH_2Cl_2, Me_2CO. Mp 290-292°. Dissoc. in DMSO soln.

Lobbia, G.G. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1987, **17**, 909 (*synth, ir, pmr, cmr, conductivity*)

IC-006805

$C_{10}H_{10}Cl_3N_2NbS$
Trichlorobis(pyridine)thioxoniobium(*V*), 11Cl
[92205-09-9]

$NbCl_3S(Py)_2$

M 389.5
Synth. from $NbCl_3S$ and Py in CH_2Cl_2. Yellow-green solid. Paramagnetic, $\mu_{eff} = 0.40\mu_B$. Ir ν_{Nb-S} 522 cm^{-1}.

bin-Baba, I., *Sains Malays.*, 1983, **12**, 249 (*synth, ir, uv-vis, magnetism*)

IC-006806

$C_{10}H_{10}Cl_3N_2ORe$
Trichlorooxobis(pyridine)rhenium(*V*), 9Cl
[18195-83-0]

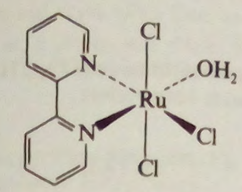
$ReOCl_3(Py)_2$

M 466.7
Geometry not established. Synth. from $ReOCl_4$ or $ReOCl_4(POCl_3)$ and Py. Green precipitate (Py).

Chakravarti, M.C., *J. Indian Chem. Soc.*, 1963, **60**, 81 (*synth*)
Johnson, N.P. *et al*, *J. Chem. Soc.*, 1964, 2614.
Guest, A. *et al*, *Can. J. Chem.*, 1971, **49**, 603 (*synth, props*)

IC-006807

$C_{10}H_{10}Cl_3N_2ORu$
Aqua(2,2′-bipyridine-*N,N′*)trichlororuthenium(*III*)
[93785-43-4]



possible structure

M 381.6
Prepd. by reducing (2,2′-Bipyridine-*N,N′*) tetrachlororuthenium(*IV*), IC-006736 with HCl/EtOH and recrystallizing from H_2O. Yellow solid. Sol. H_2O, MeOH. Yellow aq. soln. rapidly turns green.

Dwyer, F.P. *et al*, *Aust. J. Chem.*, 1963, **16**, 42 (*synth*)

IC-006808

$C_{10}H_{10}Cl_3N_3ORu$
Trichloro(nitrosyl)bis(pyridine)ruthenium, 9Cl
[15632-14-1]

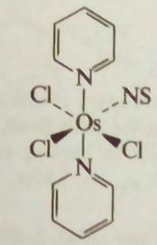
$Ru(NO)Cl_3(Py)_2$

M 395.6
Isomeric form not established; presumably similar to Tribromobis(methyldiphenylphosphine)(nitrosyl) ruthenium, IC-011876. Red cryst. Mp >320° dec. Ir ν_{NO} 1853 cm^{-1}.

Charonnat, R., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1924, **178**, 1423 (*synth*)
Charonnat, R., *Ann. Chim. (Paris)*, 1931, **16**, 217 (*synth*)
Fairy, M.B. *et al*, *J. Chem. Soc. A*, 1966, 475 (*synth, ir*)
D'yachenko, Yu.I. *et al*, *Teor. Eksp. Khim.*, 1978, **14**, 44.
Kukushkin, Yu.N. *et al*, *Zh. Neorg. Khim.*, 1983, **28**, 2858.
Nishimura, H. *et al*, *J. Chem. Soc., Dalton Trans.*, 1990, 137.

IC-006809

$C_{10}H_{10}Cl_3N_3OsS$
Trichlorobis(pyridine)(thionitrosyl)osmium
[70612-29-2]

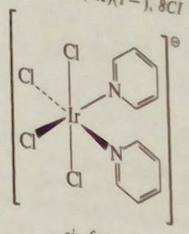


M 500.8
Synth. from S_2Cl_2, $[NBu^n_4][OsCl_4N]$ and Py. Yellow-green needles. Sol. 1,2-dichloroethane, pentane. Diamagnetic.

Bishop, M.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1 (*synth, ir*)

IC-006810

$C_{10}H_{10}Cl_4IrN_2^{\ominus}$
Tetrachlorobispyridineiridate(*III*)(1−)
Tetrachlorodipyridineiridate(III)(*1−*), *8Cl*



cis-form

M 492.2 (ion)
Octahedral.

cis-form
Pyridinium salt: [24952-68-9].
Orange cryst. Sol. H_2O.

trans-form
Pyridinium salt: [24952-67-8].
Red cryst. Spar. sol. H_2O.

Inorg. Synth., 1963, **7**, 228 (*synth*)
Herbelin, F. *et al*, *Spectrochim. Acta*, 1966, **22**, 1515 (*ir*)
Tirsell, J.B. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 2871 (*synth, kinetics*)

IC-006811

$C_{10}H_{10}Cl_4N_2O_2Th$
Tetrachlorobis(pyridine-1-oxide-*O*)thorium(*IV*)
Thorium(IV) *chloride bis(pyridine 1-oxide)*
[86349-78-2]

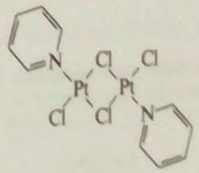
$(C_5H_5NO)_2ThCl_4$

M 564.0
Presumed 6-coord. White cryst. Sl. sol. $PhNO_2$, C_6H_6. Similar compds. obt. for substd. pyridine N-oxides. Dec. >190°.

Agarwal, R.K. *et al*, *Thermochim. Acta*, 1983, **63**, 363 (*synth, ir*)

IC-006812

$C_{10}H_{10}Cl_4N_2Pt_2$
Di-μ-chlorodichlorobis(pyridine)diplatinum(*II*), 11Cl
Tetrachlorobis(pyridine)diplatinum(II)
[66069-01-0]



M 690.1
sym-trans-form only known isomer, solubilities given are those found by Kong which differ from props. found by Allen. Reddish-yellow cryst. Sol. $CHCl_3$, Me_2CO, THF; insol. H_2O, reacts with Py, DMF. Mp 185° (170° dec.).

[57862-88-1]

Allen, A.D. *et al*, *Can. J. Chem.*, 1964, **42**, 1551 (*synth, props, ir*)
Courtot, P. *et al*, *J. Organomet. Chem.*, 1975, **99**, C59 (*synth, ir, pmr*)
Kong, P.-C. *et al*, *Can. J. Chem.*, 1979, **57**, 682 (*synth, props, ir*)

IC-006813

$C_{10}H_{10}Cl_4N_2Re$

Tetrachlorobis(pyridine)rhenium(*IV*), 8Cl

Rhenium(IV) *chloride bis(pyridine)*

[34248-13-0]

$ReCl_4(Py)_2$

M 486.2

Octahedral.

cis-form [82536-07-0]

Synth. (i) from β-$ReCl_4$ and dry Py in Me_2CO (also yields $(PyH)_2Re_2Cl_8$), (ii) by pyrolysis of $(PyH)_2ReCl_6$ in Py at 200°. Brown cryst. solid (Py). Sol. Me_2CO, Py.

Chakravarti, M.C., *J. Indian Chem. Soc.*, 1965, **42**, 503 (*synth, props*)
Tronev, V.G., *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 1351 (*synth, props, struct*)
Walton, R.A., *Inorg. Chem.*, 1971, **10**, 2534 (*synth, ir, uv, props*)
Levanda, O.Yu. *et al*, *Zh. Neorg. Khim.*, 1985, **30**, 930; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1985, **30**, 522 (*synth, ir, struct*)

IC-006814

$C_{10}H_{10}Cl_4N_2Ru^{\ominus}$

Tetrachlorobis(pyridine)ruthenate(*III*)(1−), 9Cl

[74077-62-6]

$[RuCl_4(Py)_2]^{\ominus}$

M 401.0 (ion)

Isomeric form not established. Prepd. by treating Hexachlororuthenate(*IV*)(2−), IC-017348 with Py in aq. HCl.

Pyridinium salt: Orange cryst. Mp 255° dec.

Souček, J., *Collect. Czech. Chem. Commun.*, 1962, **27**, 960 (*synth*)

IC-006815

$C_{10}H_{10}Cl_4N_2Ta$

Tetrachlorobis(pyridine)tantalum(*IV*)

Tantalum(IV) *chloride bis-pyridine*

$(Py)_2TaCl_4$

M 480.9

Octahedral: detailed geometry is not known. Synth. from $TaCl_5$ with excess Py at 50° for many days. Purple solid. Paramagnetic, $\mu_{eff} = 0.69\mu_B$, obeys Curie law.

McCarley, R.E. *et al*, *Inorg. Chem.*, 1963, **2**, 547 (*synth, struct*)
Allbutt, M. *et al*, *J. Less-Common Met.*, 1964, **6**, 299 (*synth, ir, uv-vis*)

IC-006816

$C_{10}H_{10}Cl_4N_2Tc$

Tetrachlorobis(pyridine)technetium(*IV*), 10Cl

Technetium(IV) *chloride bis(pyridine)*

[69182-24-7]

$TcCl_4(Py)_2$

M 398.9

cis-Geometry established from ir spectrum. Synth. by heating $(PyH)_2[TcCl_6]$ at 300° in a stream of Ar, or from $TcCl_4(PPh_3)_2$ + pyridine. Dark mustard solid, stable to 400° substitution-inert, paramagnetic. Almost insol. org. solvs.; spar. sol. H_2O.

[96444-37-0]

Oblova, A.A. *et al*, *Zh. Neorg. Khim.*, 1978, **23**, 3265; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1978, **23**, 1811 (*synth, ir, dta, struct*)
Gerasimov, V.N. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1982, **266**, 148 (*pe*)

Levanda, O.Yu. *et al*, *Zh. Neorg. Khim.*, 1985, **30**, 930; *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1985, **30**, 522 (*synth, ir, thermal props, magnetism, struct*)
Breikss, A.I. *et al*, *Inorg. Chim. Acta*, 1990, **170**, 75 (*synth, ir*)

IC-006817

$C_{10}H_{10}Cl_4N_2Ti$

Tetrachlorobis(pyridine)titanium(*IV*), 11Cl

Titanium(IV) *chloride bis(pyridine)*

[17100-05-9]

Py_2TiCl_4

M 347.8

Octahedral. Used in ethylene polym. and olefin conversion.

cis-form

Synth. by reaction of excess $TiCl_4$ with Py. Excess Py causes product to dec. Yellow solid.

Fowles, G.W.A. *et al*, *J. Chem. Soc.*, 1963, 33 (*synth*)
Beattie, I.R. *et al*, *J. Chem. Soc.*, 1964, 3507 (*far ir*)
Singh, S.S. *et al*, *Indian J. Chem.*, 1969, **7**, 812 (*synth, ir*)
Pomogailo, A.D. *et al*, *Vysokomol. Soedin., Ser. A*, 1971, **13**, 1931; *CA*, **76**, 15011x (*use*)
U.S. Pat., 3 670 043, (1972); *CA*, **77**, 100716w (*use*)
Cooney, R.P. *et al*, *Aust. J. Chem.*, 1974, **27**, 1855 (*raman, ir*)

IC-006818

$C_{10}H_{10}Cl_4N_2U$

Tetrachlorobis(pyridine)uranium(*IV*)

Uranium(IV) *chloride bis(pyridine)*

[12083-55-5]

UCl_4Py_2

M 538.0

Presumed 6-coord. Hygroscopic pale green or grey solid. Ir ν_{U-Cl} 280 cm^{-1} (nujol). Paramagnetic: $\mu_{eff} = 2.61\ 1\mu_B$ (θ −148°).

Selbin, J. *et al*, *J. Inorg. Nucl. Chem.*, 1966, **28**, 1385 (*synth, uv, ir*)
Gans, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1738 (*synth, ir, uv*)

IC-006819

$C_{10}H_{10}Cl_4N_2V$

Tetrachlorobis(pyridine)vanadium(*IV*), 11Cl

Vanadium(IV) *chloride bis-pyridine*

[18726-14-2]

$VCl_4(Py)_2$

M 350.9

Octahedral. Detailed geometry is unknown. Synth. by adding Py to VCl_4 in toluene. Brick red solid; readily hydrol. Forms VCl_3Py on heating to 174°. Subl. 132° *in vacuo*. Paramagnetic, $\mu_{eff} = 1.80\mu_B$ (293K). ΔH_f −190 kJ mol^{-1}.

Sarju, P. *et al*, *Indian J. Chem.*, 1965, **3**, 87 (*synth, ir*)
Kilty, P.A. *et al*, *J. Chem. Soc.*, 1965, 4915 (*synth, magnetism, thermal dec*)
Tsvetkov, V.G. *et al*, *Tr. Khim. Khim. Tekhnol.*, 1974, 83; *CA*, **82**, 65232q (*thermochem*)

IC-006820

$C_{10}H_{10}Cl_4N_2W^{\ominus}$

Tetrachlorobis(pyridine)tungstate(*III*)(1−)

As Tetrabromobis(pyridine)tungstate(*III*)(1−), IC-006783 with

X = Cl

M 483.8 (ion)

Octahedral.

trans-form

W—Cl 242.6-244.1; W—N 218.0 pm.

Pyridinium salt: [106293-40-7].

Synth. by redn. of WCl_4Py_2 by Py in 2-propanol with $NaBH_4$. V. air-sensitive violet cryst.

Pyridinium salt, Py compd.: [106293-41-8].

Air-sensitive red cryst. (Py). Dec. to 1:1 complex at r.t.

Brencic, J.V. *et al*, *Z. Anorg. Allg. Chem.*, 1986, **538**, 212 (*cryst struct, synth*)

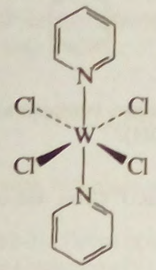
IC-006821

$C_{10}H_{10}Cl_4N_2W$

Tetrachlorobis(pyridine)tungsten(*IV*), 11Cl, 10Cl, 8Cl

Tungsten(IV) *chloride bis(pyridine)*

[20555-48-0]



M 483.8

Octahedral. Analogues with substituted pyridines also known.

trans-form [71697-95-5]

Synth. from Tetrachlorobis(triphenylphosphine) tungsten(*IV*), IC-013236 + Py, or from $W(CO)_4Cl_2$ in Py, or by reduction of WCl_6 by Py. Brown cryst. (Py). Sol. Py. $\mu_{eff} = 1.29\mu_B$ (r.t.). Non-electrolyte in Py.

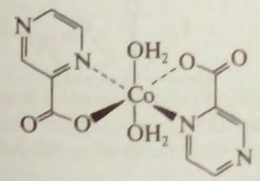
Blight, D.G. *et al*, *J. Chem. Soc. A*, 1968, 534 (*vis, magnetism, ir, synth*)
Westland, A.D. *et al*, *Inorg. Chem.*, 1973, **12**, 2356 (*synth*)
Brencic, J.V. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **454**, 181 (*cryst struct, synth, ir*)
Chatt, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 345 (*synth, reactions*)

IC-006822

$C_{10}H_{10}CoN_4O_6$

Diaquabis(2-pyrazinecarboxylato-N^1,O^2)cobalt(*II*), 10Cl

[74184-89-7]



M 341.1

Octahedral, only *trans*-config. known. Paramagnetic.

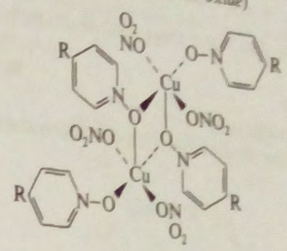
O'Connor, C.J. *et al*, *Inorg. Chem.*, 1981, **20**, 545 (*synth, struct, magnetism*)

IC-006823

$C_{10}H_{10}CuN_4O_8$

Bis(nitrato)bis(pyridine *N*-oxide)copper(*II*)

Copper(II) *nitrate bis(pyridine N-oxide)*



dimer

R = H

M 377.7

Bi-square pyramidal dimer.

Dimer: [26507-58-4]. *Tetrakis(nitrato-O)bis[μ-(pyridine 1-oxide-O:O)]bis(pyridine 1-oxide-O)dicopper(II)*, 9Cl

$C_{20}H_{20}Cu_2N_8O_{16}$ M 755.5

Obt. by mixing EtOH solns. of $Cu(NO_3)_2 \cdot 3H_2O$ and pyridine 1-oxide. Emerald green cryst. Cu...Cu 345.8 pm.

Quagliano, J.V. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 3770 (*synth, ir*)
Scavnicar, S. *et al*, *Acta Crystallogr., Sect. B*, 1969, **25**, 2046 (*cryst struct*)
Boyd, P.D.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1549 (*esr*)

IC-006824

$C_{10}H_{10}HgN_2^{2\oplus}$

Bis(pyridine)mercury(*II*)(2+)

Dipyridinemercury(2+)

[41290-90-8]

$(Py)_2Hg^{2\oplus}$

M 358.7 (ion)

N-Hg-N moiety is linear.

Dinitrate: [59244-53-0]. *Mercury*(II) *nitrate bis(pyridine)*

Cryst. Forms a dihydrate.

Diperchlorate: [25770-72-3]. *Mercury*(II) *perchlorate bis(pyridine)*

Cryst. (MeOH or MeCN).

▷ Potentially explosive.

[59244-54-1]

Chudimova, L.I. *et al*, *Zh. Neorg. Khim.*, 1969, **14**, 2974; 1973, **18**, 47 (*ir*)
Kamenar, B. *et al*, *Cryst. Struct. Commun.*, 1976, **5**, 149 (*cryst struct*)
Tan, K.-H. *et al*, *Aust. J. Chem.*, 1980, **33**, 1753 (*synth, ir, raman*)
Bowmaker, G.A. *et al*, *J. Chem. Res. (S)*, 1984, 158 (*synth*)
Hulten, F. *et al*, *Inorg. Chim. Acta*, 1987, **127**, L33 (*stability const*)

IC-006825

$C_{10}H_{10}I_2N_2Pt$

Diiodobis(pyridine)platinum(*II*), 8Cl

[32162-03-1]

As Dibromobis(pyridine)platinum(*II*), IC-006780 with

X = I

M 607.0

cis-form [15227-45-9]

Yellow needles. Sol. many org. solvs. Solns. slowly dec. to *trans*-isomer.

trans-form [15227-44-8]

More stable form. Bright yellow prisms. Sol. org. solvs.

Durig, J.R. *et al*, *Spectrochim. Acta, Part A*, 1967, **23**, 1121 (*synth, ir*)

Haake, P. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 6823 (*ms*)
Texter, M. *et al*, *Helv. Chim. Acta*, 1972, **55**, 184 (*ur*)
Thiele, G. *et al*, *Chem. Ber.*, 1978, **111**, 3162 (*struct*)
Dickinson, R.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 895 (*mössbauer*)
Kravchenko, E. *et al*, *J. Mol. Struct.*, 1982, **83**, 163 (*ngr*)

IC-006826

$C_{10}H_{10}I_2N_2Zn$
Diiodobis(pyridine)zinc
Bis(pyridine)zinc diiodide. Zinc(II) *iodide bis(pyridine)*
[14025-05-9]

$(Py)_2ZnI_2$

M 477.4
White cryst. Mp 205°.

Clark, R.J.H. *et al*, *Inorg. Chem.*, 1965, **4**, 350 (*ir*)
Graddon, D.P. *et al*, *Aust. J. Chem.*, 1966, **19**, 1801 (*synth, ir*)
Allan, J.R. *et al*, *J. Chem. Soc. A*, 1966, 1031 (*synth, ir*)
Liptay, G. *et al*, *J. Therm. Anal.*, 1970, **2**, 25 (*thermal, anal*)
Saito, Y. *et al*, *Spectrochim. Acta, Part A*, 1972, **28**, 1459 (*ir*)
LeQuerler, J.F. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 2299 (*cryst struct*)
Hsieh, Yu.-N. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 1384 (*N-14 nqr*)
Hutton, A.T. *et al*, *Spectrosc. Lett.*, 1977, **10**, 57 (*ir*)

IC-006827

$C_{10}H_{10}I_2N_2ORu$
Diiodo(nitrosyl)bis(pyridine)ruthenium, 9CI
[15708-23-3]

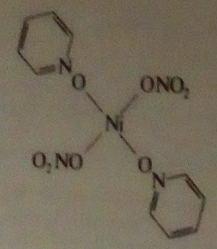
$[Ru(NO)I_2(Py)_2]_n$ $(n \geqslant 2)$

M 543.0
Probably dimeric. Prepd. by treating Diiodo(nitrosyl) ruthenium, IC-020215 with boiling Py. Air-stable red solid, showing small temp. independent paramagnetism. Ir ν_{NO} 1823, 1784 cm^{-1}.

Irving, R.J. *et al*, *J. Chem. Soc. A*, 1966, 161 (*synth, ir*)

IC-006828

$C_{10}H_{10}N_4NiO_8$
Bis(nitrato-*O*)bis(pyridine-1-oxide)nickel(*II*)
Dinitratobis(pyridine-N-oxide)nickel(II)

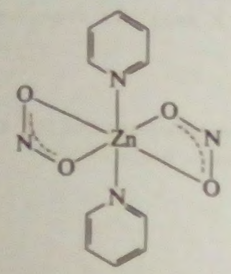


M 372.9
Light-green solid. Mp 230-232°.

Carlin, R.L. *et al*, *J. Chem. Soc.*, 1964, 5008 (*synth, ir, ue*)

IC-006829

$C_{10}H_{10}N_4O_4Zn$
Bis(nitrito-*O*)bis(pyridine)zinc
Bis(pyridine)zinc dinitrite. Zinc(II) *nitrite bis(pyridine)*
[88437-50-7]



M 315.6
Monomeric in solid state, contains asymmetrically bonded $NO_2^{\ominus}$. Cryst. (EtOH).

[29855-53-6]

Goodgame, D.M.L. *et al*, *J. Chem. Soc. A*, 1970, 1933 (*synth*)

IC-006830

$C_{10}H_{10}N_4O_6Zn$
Bis(nitrato-*O*)bis(pyridine)zinc(*II*)
Bis(pyridine)zinc dinitrate
[25754-93-2]

$(Py)_2Zn(ONO_2)_2$

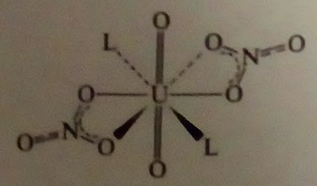
M 347.6
Tetrahedral zinc. Cryst. (EtOH/$(MeO)_2CHCH_2CH_3$/Py).

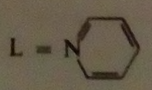
[22972-23-2]

Ouellette, T.J. *et al*, *Inorg. Chem.*, 1969, **8**, 1777 (*synth, ir*)
Nuttall, R.H. *et al*, *J. Chem. Soc. A*, 1971, 3103 (*synth, ir*)
Cameron, A.F. *et al*, *J. Chem. Soc. A*, 1971, 3402 (*cryst struct*)
Hsieh, Yu.-N. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 1384 (*N-14 nqr*)
Rubenacker, G.V. *et al*, *Inorg. Chem.*, 1980, **19**, 392 (*N-14 nqr*)

IC-006831

$C_{10}H_{10}N_4O_8U$
Dioxobis(nitrato-*O,O'*)bis(pyridine)uranium(*VI*)
Uranyl nitrate bis(pyridine)
[18077-76-4]





M 552.2
8-Coord. hexagonal bipyramid. Bright yellow cryst. Sol. MeOH, EtOH, Me_2CO. Cryst. lose Py when exposed to air and *in vacuuo*.

Barr, H. *et al*, *J. Am. Chem. Soc.*, 1952, **74**, 4430 (*synth, ir*)
Pennington, M. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 1664 (*cryst struct*)

IC-006832

$C_{10}H_{10}N_6O_2S_6Ti_2$
Diethoxybis[μ-(thiocyanato-*N*:*S*)]tetrakis(thiocyanato-*N*) dititanium(*IV*), 11CI
[92181-97-0]

$Ti_2(\mu\text{-}SCN)_2(NCS)_4(OEt)_2$

M 534.3
Octahedral dimer, detailed geometry not known. Synth. from $Ti(OEt)_4$ and AgNCS.

Gorsi, B.L. *et al*, *J. Indian Chem. Soc.*, 1984, **61**, 189 (*synth, ir*)

IC-006833

$C_{10}H_{10}N_6O_{12}Th$
Tetrakis(nitrato-*O,O'*)bis(pyridine)thorium(*IV*), 10CI
Thorium(IV) *nitrate bis(pyridine)*
[77306-34-4]

$Th(NO_3)_4Py_2$

M 638.2
Presumed 10-coord. with bidentate nitrates. White cryst. Sol. $PhNO_2$.

*Bis-*N*-oxide:* [85159-61-1]. *Tetrakis(nitrato-*O,O') *bis(pyridine-1-oxide-*O)*thorium*(IV)
$C_{10}H_{10}N_6O_{14}Th$ M 670.2
White cryst. (EtOAc). Sl. sol. EtOAc, sol. DMF. Dec. >200°. Presumed 10-coord.

Agarwal, R.K. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **42**, 1775 (*synth, ir*)
Wassef, M.A. *et al*, *Acta Chim. Acad. Sci. Hung.*, 1982, **111**, 199 (*synth, ir*)

IC-006834

$C_{10}H_{10}N_8Zn$
Diazidobis(pyridine)zinc
Bis(pyridine)zinc diazide. Zinc(II) *azide bis(pyridine)*
[30105-21-6]

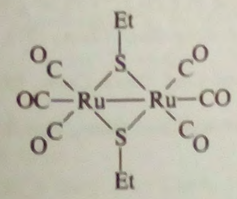
$Zn(N_3)_2(Py)_2$

M 307.6
Tetrahedral at Zn. Colourless needles, unstable in air.

Dennis, L.M. *et al*, *J. Am. Chem. Soc.*, 1907, **29**, 21.
Strecker, W. *et al*, *J. Prakt. Chem.*, 1939, **152**, 212.
Agrell, I., *Acta Chem. Scand.*, 1970, **24**, 1247; 1971, **25**, 2965 (*synth, cryst struct, ir*)

IC-006835

$C_{10}H_{10}O_6Ru_2S_2$
Hexacarbonylbis-μ-(ethanethiolato)diruthenium
Bis-μ-ethanethiolato-bis[tricarbonylruthenium(I)].
Hexacarbonyldiethyldi-μ-thiodiruthenium(I), *8CI*
[15556-31-7]

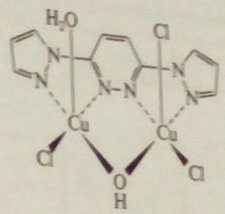


M 492.4
Tentative struct. shown. Prepd. by treating Dodecacarbonyltriruthenium, IC-008378 with either EtSH or Et_2S_2. Air-stable brown solid. Sol. CCl_4, $CHCl_3$, CH_2Cl_2. Mp 67-68°. Ir ν_{CO} 2084, 2061, 2025, 2017, 1998, 1933 cm^{-1} (CCl_4).

Johnson, B.F.G. *et al*, *Nature* (*London*), 1967, **213**, 901 (*synth*)
Cetini, G. *et al*, *J. Organomet. Chem.*, 1968, **15**, P4 (*synth, ir*)

IC-006836

$C_{10}H_{11}Cl_3Cu_2N_6O_2$
Aquatrichloro[μ-(3,6-di-1*H*-pyrazol-1-ylpyridazine)]-μ-hydroxydicopper, 11CI
[μ-3,6-Bis(1-pyrazolyl)pyridazine-N^1,μ-N^2,μ-N^4,N^5](μ-hydroxo)trichlorooaquodicopper
[106589-97-3]

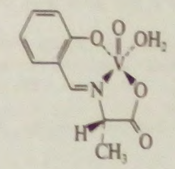


M 480.6
A binuclear copper protein analogue. Green cryst. + $0.8H_2O$.

Thompson, L.K. *et al*, *Inorg. Chem.*, 1985, **24**, 4719; 1987, **26**, 657 (*synth, cryst struct, magnetism, electrochem*)

IC-006837

$C_{10}H_{11}NO_5V$
Aquaoxo[*N*-salicylidene-L-alaninato(2–)]vanadium(*IV*), 8CI
Aqua[N-[(2-*hydroxyphenyl*)*methylene*]-L-*alaninato*(2–)-N,O,O^x]*oxovanadium*(IV), *11CI*
[99880-77-0]



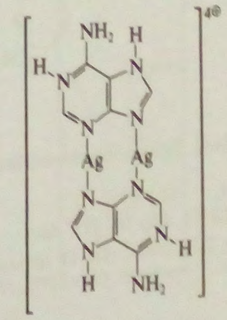
M 276.1
Square pyramidal. Synth. by refluxing alanine and salicylaldehyde in EtOH then adding $VOSO_4.5H_2O$ and NaOH in H_2O. Green solid.

[25807-26-5, 25807-27-6, 30934-43-1, 86593-41-1]

Theriot, L.J. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 2840 (*synth, uv-vis*)
Frausto da Silva, J.J.R. *et al*, *J. Chem. Soc. A*, 1970, 3369 (*synth*)
Hämäläinen, R. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 1726 (*synth, cryst struct*)

IC-006838

$C_{10}H_{12}Ag_2N_{10}^{4\oplus}$
Di-μ-(adeninium)disilver(*I*)(4+)



M 488.0 (ion)

Tetraperchlorate: [63301-89-3]. *Bis[μ-(1H-purin-6-amine-N¹,N⁶)]disilver(2+), diperchlorate, diperchlorate, 10Cl*
Colourless cryst. + $2H_2O$.

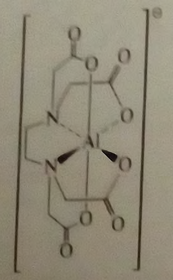
Gagnon, C. *et al, Inorg. Chem.*, 1977, **16**, 2469 (*synth, cryst struct*)

IC-006839

$C_{10}H_{12}AlN_2O_8^{\ominus}$

(Ethylenediaminetetraacetato-*O,O',O'',O'''*)aluminate(1−)
Aluminium ethylenediaminetetraacetate. [N,N-*1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinato*(*4*−)]]*aluminate*(*1*−). *Aluminium (EDTA)*

[15009-37-7]



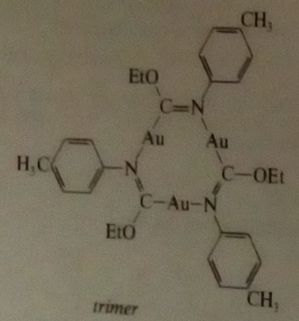
M 315.1 (ion)
Log K_1 16.7 (I = 0.1).
K salt: [12558-45-1].
Colourless cryst. + $2H_2O$.

Schwarzenbach, G. *et al, Helv. Chim. Acta*, 1948, **31**, 459 (*potent titration*)
Anderegg, G., *Critical Survey of Stability Constants of EDTA Complexes*, Pergamon, Oxford, 1967 (*thermodyn*)
Polynova, T.N. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1970, **11**, 158 (*cryst struct*)
Tsuchimoto, M. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 717 (*reaction*)

IC-006840

$C_{10}H_{12}AuNO$

[Ethoxy(*p*-tolylimino)methyl-*C,N*]gold(*I*)



trimer

M 359.1
Trimeric.

Trimer: [55145-58-9]. *Tris-μ-[ethoxy(*p*-tolylimino)methyl-C,N]trigold*
$C_{30}H_{36}Au_3N_3O_3$ M 1077.5
Needles. Sol. $CHCl_3$. Mp 181-183° dec.

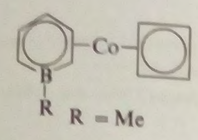
Minghetti, G. *et al, Inorg. Chem.*, 1974, **13**, 1600 (*synth*)
Tiripicchio, A. *et al, J. Organomet. Chem.*, 1979, **171**, 399 (*synth, cryst struct*)

IC-006841

$C_{10}H_{12}BCo$

Cyclobutadiene(1-methylborinato)cobalt
(η⁴-*1,3-Cyclobutadiene*)[*methyl*(η⁵-*1,3-pentadien-1-yl-5-ylidene*)*borato*(*1*−)-B]*cobalt, 11Cl. Cyclobutadiene(1-methyl-1-boratabenzene)cobalt*

[95407-79-7]



R = Me

M 201.9
Orange-red oil, essentially stable to air. Sol. $CHCl_3$. $Bp_{0.00001}$ 60°. ^{11}B nmr δ 24.0.

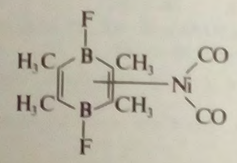
Herberich, G.E. *et al, J. Organomet. Chem.*, 1985, **280**, 147 (*synth, nmr, ms*)
Böhm, M.C. *et al, J. Phys. Chem.*, 1985, **89**, 2129.

IC-006842

$C_{10}H_{12}B_2F_2NiO_2$

Dicarbonyl[(2,3,5,6-η)-1,4-difluoro-1,4-dihydro-2,3,5,6-tetramethyl-1,4-diborin]nickel

[56978-08-6]



M 282.5
Yellow, air-sensitive cryst. Sol. CCl_4.

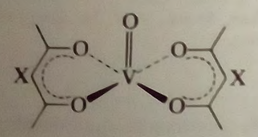
Maddren, P.S. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 1272 (*synth, ir, raman, nmr, ms*)

IC-006843

$C_{10}H_{12}Br_2O_5V$

Bis(3-bromo-2,4-pentanedionato-*O,O'*)oxovanadium(*IV*), 11Cl
Bis(*3-bromoacetylacetonato*)*oxovanadium*(IV)

[70289-80-4]



X = Br

M 422.9
Prob. square pyramidal. Synth. from $VO(acac)_2$ and *N*-bromosuccinimide in $CHCl_3$. Yellow-green solid.

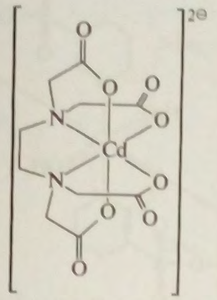
Mannix, C.E. *et al, J. Inorg. Nucl. Chem.*, 1979, **41**, 59 (*synth, uv-vis, ir*)
Vlckova, B. *et al, Proc. Conf. Coord. Chem.*, 9th, 1983, 455 (*ir, raman*)
Sing, V. *et al, J. Macromol. Sci., Chem., Part A*, 1985, **22**, 33 (*dipole moment*)

IC-006844

$C_{10}H_{12}CdN_2O_8^{2\ominus}$

(Ethylenediaminetetraacetato)cadmate(2−)
[[N,N'-*1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4*−)-N,N',O,O',O^N,O^N]*cadmate*(*2*−), *9Cl*. [(*Ethylenedinitrilo*)*tetraacetato*]*cadmate*(*2*−), *8Cl*

[36077-58-4]



M 400.6 (ion)
Di-Na salt: [35803-35-1]. *Disodium cadmium EDTA*
Cryst. (aq. EtOH).

[14972-98-6]

Sawyer, D.T. *et al, J. Am. Chem. Soc.*, 1959, **81**, 816 (*synth, ir*)
Day, R.J. *et al, Anal. Chem.*, 1965, **37**, 1326 (*pmr*)
Howarth, O.W. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 2271 (*cmr*)
Mennitt, P.G. *et al, J. Phys. Chem.*, 1981, **85**, 2087 (*Cd-113 nmr*)

IC-006845

$C_{10}H_{12}Cl_2N_2O_8Ru^{2\ominus}$

Dichloro(ethylenediaminetetraacetato)ruthenate(*IV*)(2−)
Dichloro[[N,N'-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4*−)-N,N',O,O']*ruthenate*(*2*−), *9Cl*

$RuCl_2[(OOCCH_2)_2NCH_2CH_2N(CH_2COO)_2]^{2\ominus}$

M 460.1 (ion)
Six-coordinate complex; struct. undetermined.
Di-K salt: Prepd. by treating $K_2[RuCl_6]$ with $Na_2[H_2edta]$, followed by KOAc. Violet solid + $3H_2O$.
Di-NH_4 salt: Synth. analogous to K salt. Violet solid + $2H_2O$.

Scherzer, J. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 1107 (*synth*)

IC-006846

$C_{10}H_{12}Cl_2O_5V$

Bis(3-chloro-2,4-pentanedionato-*O,O'*)oxovanadium(*IV*), 11Cl
Bis(*3-chloroacetylacetonato*)*oxovanadium*(IV)

[19788-13-7]

As Bis(3-bromo-2,4-pentanedionato-*O,O'*) oxovanadium(*IV*), IC-006843 with

X = Cl

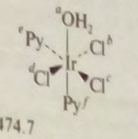
M 334.0
Synth. from $VO(acac)_2$ and *N*-chlorosuccinimide in $CHCl_3$. Yellow-green solid.

Mannix, C.E. *et al, J. Inorg. Nucl. Chem.*, 1979, **41**, 59 (*synth, uv-vis, ir*)
Adeleke, B.B. *et al, J. Coord. Chem.*, 1982, **11**, 201 (*esr*)
Milani, F. *et al, Inorg. Chim. Acta*, 1985, **103**, 15 (*use*)
Singh, V. *et al, J. Macromol. Sci., Chem., Part A*, 1985, **22**, 33 (*dipole moment*)

IC-006844 – IC-006849

$C_{10}H_{12}Cl_3IrN_2O$

Aquatrichlorobis(pyridine)iridium(*III*)



a-aqua-b,c,d,-trichloro-form

M 474.7
Octahedral, several isomers known.

a-aqua-b,c,d-trichloro-form
mer, cis-*form*
Prepd. by irradiation of *cis*-$K[IrPy_2Cl_4].H_2O$ in soln. in sunlight. Orange-yellow solid. Sol. H_2O.

a-aqua-b,c,f-trichloro-form [17458-72-9]
fac, cis-*form*
Prepd. by treating *cis*-$(NH_4)[IrPy_2Cl_4]$ with Py at 110°. Orange-yellow solid. Sol. H_2O.

a-aqua-b,d,f-trichloro-form [24952-69-0]
mer,trans-*form*
Orange-red solid. Sol. H_2O.

Delépine, M., *Compt. Rend. Hebd. Seances Acad. Sci.*, 1956, **242**, 27 (*synth*)
Tirsell, J.B. *et al, J. Inorg. Nucl. Chem.*, 1969, **31**, 2871 (*synth, uv, kinetics*)

IC-006848

$C_{10}H_{12}Cl_6N_2Tc$

Pyridinium hexachlorotechnetate(*IV*)

[40888-87-7]

$(PyH)_2TcCl_6$

M 471.8
Synth. by metathesis from K_2TcCl_6. Yellow-green cryst. On heating above 250° Py begins to displace $Cl^{\ominus}$; above 300° $TcCl_4(Py)_2$ is produced. μ_{eff} = 3.97 μ_B.

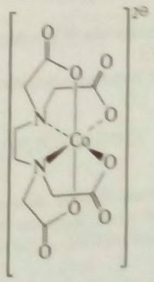
Kuzina, A.F. *et al, Zh. Neorg. Khim.*, 1972, **17**, 2630; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1972, **17**, 1377 (*synth, powder struct*)
Zelentsov, V.V. *et al, Zh. Neorg. Khim.*, 1973, **18**, 1709; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 902 (*magnetism*)
Oblova, A.A. *et al, Zh. Neorg. Khim.*, 1978, **23**, 3265; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1978, **23**, 1811 (*powder struct, thermal dec*)

IC-006849

$C_{10}H_{12}CoN_2O_8^{2\ominus}$

(Ethylenediaminetetraacetato)cobaltate(*II*)(2−)
(*Edta*)*cobaltate*(*2*−)

[14931-83-0]



M 347.1 (ion)
Tetraaquacobalt(2+) salt: [12785-79-4].
$C_{10}H_{28}Co_2N_2O_{12}$ M 478.1

Pink cryst. + $2H_2O$. Sol. hot H_2O. Contains 6-coord. Co in both cation and anion in polymeric struct.

Im, Y.A. *et al, J. Am. Chem. Soc.*, 1961, **83**, 3357 (*reaction*)
Rosenheim, L. *et al, Inorg. Chem.*, 1974, **13**, 1571 (*reaction*)

$C_{10}H_{12}CrN_2O_8^{2\ominus}$ IC-006850

(Ethylenediaminetetraacetato)chromate(*II*)(2−)
[[N,N′-1,2-Ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N′,O,O′,O^N,O$^{N'}$]chromate(2−), 11CI, 10CI, 9CI.
[(Ethylenedinitrilo)tetraacetato]chromate(2−), 8CI

[12558-56-4]

$[[(OOCCH_2)_2NCH_2CH_2N(CH_2COO)_2]Cr]^{2\ominus}$

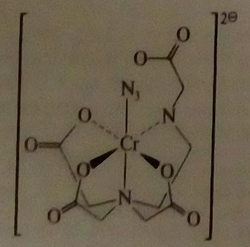
M 340.2 (ion)
Known only in aq. soln; EDTA prob. pentadentate with H_2O in 6th position. Powerful reducing agent. Log K_1 12.7 (25°, 1*M* KCl). $E°$ −1.48V (vsSCE, pH12). μ_{eff} = 5.12μ_B (293K, aq. soln.).

Pecsok, R.L. *et al, Inorg. Chem.*, 1964, **3**, 114 (*stability const*)
Henderson, R.A. *et al, Inorg. Chem.*, 1980, **19**, 3103 (*use*)
Ogino, H. *et al, Inorg. Chem.*, 1982, **21**, 126 (*kinetics*)
Micskei, K. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1335 (*stability const*)
Korsse, J. *et al, Inorg. Chim. Acta*, 1984, **88**, 67 (*electrochem*)
Rotman, A. *et al, Inorg. Chem.*, 1985, **24**, 4158 (*kinetics*)

$C_{10}H_{12}CrN_5O_8^{2\ominus}$ IC-006851

Azido(ethylenediaminetetraacetato)chromate(*III*)
Azido[[N,N′-1,2-ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N′,O,O′,O^N]chromate(III)(2−), 9CI

[55622-32-7]



M 382.2 (ion)
Formed in soln. Tentative geometry shown. Obt. reversibly on addition of azide buffer soln. to Cr(edta)$OH_2^{\ominus}$. Not isol.

Ogino, H. *et al, Inorg. Chem.*, 1975, **14**, 2093 (*formn, uv-vis*)

$C_{10}H_{12}CrN_6S_2$ IC-006852

Bis(2-methyl-1*H*-imidazole-*N*^{3})bis(thiocyanato-*S*)chromium(*II*), 10CI
Diisothiocyanatobis(2-methylimidazole)chromium(II)

[73084-91-0]

$Cr(NCS)_2(C_4H_6N_2)_2$

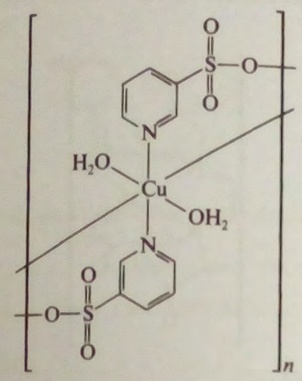
M 332.3
Polymeric 5-coordinate through thiocyanate bridges; square pyramidal struct. suggested from spectral evidence. Air-sensitive solid. μ_{eff} = 4.48 (295K); μ_{eff} = 4.06μ_B (84K).

Dapporto, P. *et al, J. Chem. Res. (S)*, 1979, 374 (*synth, magnetism, uv*)

$C_{10}H_{12}CuN_2O_8S_2$ IC-006853

Diaquabis(3-pyridinesulfonato-*O*)copper(*II*), 10CI
Copper(II) bis(pyridine-3-sulfonate) dihydrate

[74422-20-1]



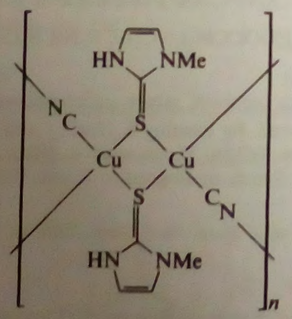
M 415.8
Contains an elongated rhombic octahedral CuN_2O_4 chromophore, with bridging pyridinesulfonate groups. Dark blue cryst.

Walsh, B. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 681 (*synth, cryst struct, esr, uv*)

$C_{10}H_{12}Cu_2N_6S_2$ IC-006854

Bis(cyano-*C*)bis[μ-(1,3-dihydro-1-methyl-2*H*-imidazole-2-thione-*S*:*S*)]dicopper
Cyano(1-methylimidazoline-2-thione)copper(I) dimer

[119654-87-4]



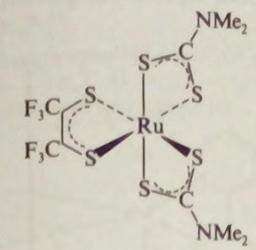
M 407.4
Dimeric units are linked via cyanide ligands to form sheet struct. Colourless cryst. (aq. soln.).

Raper, E.S. *et al, Inorg. Chim. Acta*, 1989, **155**, 77 (*synth, cryst struct, ir*)

$C_{10}H_{12}F_6N_2RuS_6$ IC-006855

Bis(dimethylcarbamodithioato-*S*,*S*′)[1,1,1,4,4,4-hexafluoro-2-butene-2,3-dithiolato(2−)-*S*,*S*′]ruthenium, 9CI
Bis(N,N-dimethyldithiocarbamato)[1,2-bis(trifluoromethyl)ethane-1,2-dithiolato]ruthenium

[51152-83-1]



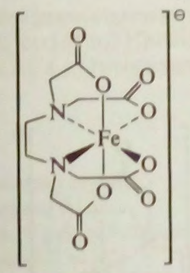
M 567.6
Although formally Ru(*IV*), this complex is diamagnetic and behaves as Ru(*II*). Prepd. by treating Dicarbonylbis[μ-(dimethylcarbamodithioato-*S*:*S*,*S*′)]bis(dimethylcarbamodithioato-*S*,*S*′)diruthenium, IC-008717 with bis(perfluoromethyl)-1,2-dithietene in THF at reflux. Violet, diamagnetic cryst. Mp 262°.

Pignolet, L.H. *et al, J. Am. Chem. Soc.*, 1971, **93**, 360 (*synth, ir, pmr*)
Pignolet, L.H. *et al, Inorg. Chem.*, 1974, **13**, 1263 (*electrochem*)

$C_{10}H_{12}FeN_2O_8^{\ominus}$ IC-006856

(Ethylenediaminetetraacetato)ferrate(*III*)(1−)
[[N,N′-Ethanediylbis[N-(carboxymethyl)glycinato](4−)-N,N′,O,O′,O^N,O$^{N'}$]ferrate(1−), 11CI. Ferric edetate

[15275-07-7]



M 344.0 (ion)
Octahedral anion, but usually obt. with coordinated H_2O see Aqua(ethylenediaminetetraacetato)ferrate(*III*)(1−), IC-006910. Iron source for diet and agriculture; oxidation and photo-catalyst; redox agent; DNA cleavage.

Na salt: [15708-41-5]. *Ferric sodium edate. Sodium feredetate. Ferrostrane. Ferrostrene. Sybron*
Photographic bleach; commercially available. Used in treatment of anaemia. Cryst. (EtOH aq.). Salts with other alkali metals also known.
▷ AH4900000.

H compd.: [17099-81-9].
Anticatalyst, photographic bleach, used in fuel cells, oxidation.
▷ NO6880000.

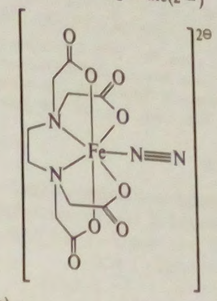
NH_4 salt: [21265-50-9].
Photographic bleaching agent.

[18154-32-0, 85528-55-8]

Takeda, M., *Hyperfine Interact.*, 1986, **28**, 737; *CA*, **105**, 90029e (*mössbauer*)

$C_{10}H_{12}FeN_4O_8^{2\ominus}$ IC-006857

(Dinitrogen)[ethylenediaminetetraacetato(4−)]ferrate(*II*)(2−)
(Dinitrogen)[[N,N′-1,2-ethanediylbis(N-carboxymethyl)glycinato](4−)-N,N′,O,O′,O^N]ferrate(2−)



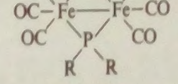
M 372.0 (ion)
Diamagnetic. Synth. from [Fe(H edta)(H_2O)] + NaN_3.
Di-Na salt: [91185-44-3].
Orange brown cryst. + $2H_2O$. Loses N_2 upon attempted recryst. Ir $\nu_{N\equiv N}$ 2040 cm^{-1}.

Lopez-Alcala, J.M. *et al, Polyhedron*, 1984, **3**, 623 (*synth, ir, thermal behaviour*)
Inorg. Synth., 1986, **24**, 208 (*synth*)

$C_{10}H_{12}Fe_2O_6P_2$ IC-006858

Hexacarbonylbis[μ-(dimethylphosphino)]diiron, 9CI

[14871-43-3]



R = Me

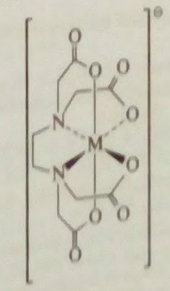
M 401.8
Yellow or orange cryst. (C_6H_6/hexane or CH_2Cl_2/hexane). Mp 221.5-222°, Mp 216-217°. $Subl._{0.1}$ 90°.

Hayter, R.G., *Inorg. Chem.*, 1964, **3**, 711 (*synth, ir, pmr*)
Johnson, B.F.G. *et al, J. Chem. Soc. A*, 1967, 1445 (*ms*)
Dessy, R.E. *et al, J. Am. Chem. Soc.*, 1972, **94**, 746 (*pmr*)
Adams, R.D. *et al, Inorg. Chem.*, 1975, **14**, 1395 (*synth, pmr, cmr*)

$C_{10}H_{12}GaN_2O_8^{\ominus}$ IC-006859

(Ethylenediaminetetraacetato)gallate(1−)
[N,N-1,2-Ethanediylbis[N-(carboxymethyl)glycinato(4−)]][gallate(1−), 9CI. Gallium(EDTA)$^{\ominus}$

[14947-72-9]



M = Ga

M 357.9 (ion)

A range of cryst. salts and hydrates descr. Log K 21.1, I 0.1 *M*.

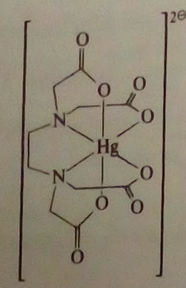
H compd., monohydrate: [67840-47-5].
$C_{10}H_{14}GaN_2O_9$ M 376.9
Synth. from $Ga(NO_3)_3$, NaEDTA, $HClO_4$. Colourless cryst. (aq. Me_2CO). Sol. H_2O; spar. sol. Me_2CO.
K salt, trihydrate: Colourless cryst. (aq. Me_2CO).

Saito, K. *et al, J. Chem. Soc.*, 1956, 4701 (*synth, titrations*)
Anderegg, G., *Critical Survey of Stability Constants of EDTA Complexes*, Pergamon, Oxford, 1967 (*thermodyn*)
Bottari, E. *et al, Helv. Chim. Acta*, 1967, **50**, 2349 (*titrations*)

$C_{10}H_{12}HgN_2O_8^{2\ominus}$ IC-006860

(Ethylenediaminetetraacetato)mercurate(2−)
[[N,N′-1,2-Ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N,O,O′,O^N,O^N]mercurate(2−), 9CI. *[(Ethylenedinitrilo)tetraacetato]mercurate(2−), 8CI*

[54735-68-1]



M 488.8 (ion)

Di-Na salt: [14689-27-1]. *Disodium mercuric EDTA*
Reagent for dehydrogenation of org. compds. Cryst. (aq. EtOH).

[14852-73-4]

Sawyer, D.T. *et al, J. Am. Chem. Soc.*, 1959, **81**, 816 (*synth, ir*)
Day, R.J. *et al, Anal. Chem.*, 1965, **37**, 1326 (*pmr*)
Moehrle, H., *Arch. Pharm.*, 1966, **299**, 529 (*synth*)
Howarth, O.W. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 2271 (*cmr*)

$C_{10}H_{12}InN_2O_8^{\ominus}$ IC-006861

(Ethylenediaminetetraacetato)indate(1−)
[N,N′-1,2-Ethanediylbis[N-(carboxymethyl)glycinato(4−)]] indate(1−), 9CI. Indium(EDTA)$^{\ominus}$

[14947-73-0]

As (Ethylenediaminetetraacetato)gallate(1−), IC-006859 with

M = In

M 403.0 (ion)
A range of cryst. salts and hydrates descr. Log K 25.3, I 0.1*M*.

H compd., monohydrate: [25429-19-0]. *Monohydrogen aquoethylenediaminetetraacetatoindium(III)*
$C_{10}H_{15}InN_2O_9$ M 450.0
Synth. from $In(OH)_3$ + EDTA + $HClO_4$. Colourless cryst. (aq. Me_2CO). Sol. H_2O; spar. sol. Me_2CO.
K salt, dihydrate: Synth. from $In(OH)_3$ + EDTA + KOH. Colourless cryst. (aq. Me_2CO).

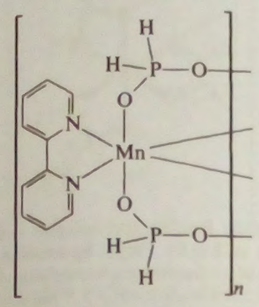
Saito, K. *et al, J. Chem. Soc.*, 1956, 4701 (*synth, titrations*)
Saito, K. *et al, J. Inorg. Nucl. Chem.*, 1963, **25**, 1245 (*synth*)
Anderegg, G., *Critical Survey of Stability Constants of EDTA Complexes*, Pergamon, Oxford, 1967 (*thermodyn*)
Bottari, E. *et al, Helv. Chim. Acta*, 1967, **50**, 2349 (*titrations*)

Tsuchimoto, M., *Bull. Chem. Soc. Jpn.*, 1975, **48**, 717 (*reactions*)
Ershova, S.D. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1988, **33**, 2245 (*synth, ir, thermal anal*)

$C_{10}H_{12}MnN_2O_4P_2$ IC-006862

(2,2′-Bipyridine-*N,N′*)bis(phosphinato-*O*)manganese(*II*), 10CI
Bis(phosphinato)(2,2′-bipyridyl)manganese(II)

[65804-80-0]



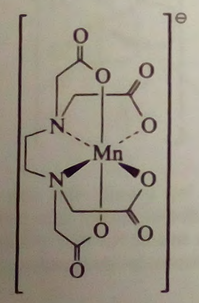
M 341.1
Polymeric chain struct. with octahedral Mn and bridging phosphinato groups. Synth. from $Mn(PH_2O_2)_2.H_2O$ in H_2O with bipy in EtOH. Yellow laths (EtOH aq.).

Sala-Pala, J. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1974, **274**, 595 (*synth*)
Weakley, T.J.R., *Acta Crystallogr., Sect. B*, 1978, **34**, 281 (*cryst struct, ir, uv, magnetism, esr*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1982, **D3**, 213 (*rev, bibl*)

$C_{10}H_{12}MnN_2O_8^{\ominus}$ IC-006863

(Ethylenediaminetetraacetato)manganate(*III*)(1−)
[[N,N′-1,2-Ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N′,O,O′,O^N,O^N]manganate(1−), 11CI

[11133-34-9]



M 343.1 (ion)
Mn—O 190, 240 pm. Previously formulated with 2.5 mol. H_2O. Synth. from freshly prepd. MnO_2 in aq. KOH with H_4edta in aq. EtOH or $Mn(acac)_3$, KOH and H_4edta.
K salt: [66615-87-0].
Air-stable red needles + $2H_2O$ (aq. EtOH); reduced by $O_2^{\ominus}$ to $[Mn^{II}(edta)]^{2\ominus}$. Sol. H_2O; sl. sol. AcOH; insol. EtOH, Me_2CO, Et_2O. Mp ~70° dec. μ_{eff} = 4.89μ_B (294 K).

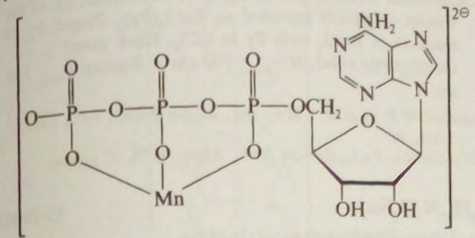
Yoshino, Y. *et al, Can. J. Chem.*, 1962, **40**, 775 (*synth, magnetism, ir*)
Hamm, R.E. *et al, Inorg. Chem.*, 1967, **6**, 139 (*synth*)
Takeuchi, T. *et al, Nippon Kagaku Kaishi (J. Chem. Soc. Jpn.)*, 1974, 1486; *CA*, 1974, **81**, 113572 (*ir*)

Lis, T., *Acta Crystallogr., Sect. B*, 1978, **34**, 1342 (*synth, cryst struct*)
Pechurova, N.I. *et al, Moscow Univ. Chem. Bull. (Engl. Transl.)*, 1978, **33**, 48 (*ir*)
Stein, J. *et al, Inorg. Chem.*, 1979, **18**, 3511 (*synth, cryst struct, uv-vis*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 51 (*rev, bibl*)

$C_{10}H_{12}MnN_5O_{13}P_3^{2\ominus}$ IC-006864

[Adenosine 5′-triphosphato(4−)-*O*^{P},*O*$^{P'}$,*O*$^{P''}$] manganate(2−), 10CI
(Adenosine triphosphate)manganate(II)

[64441-23-2]

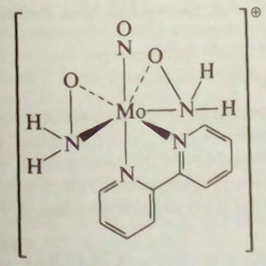


M 558.0 (ion)
Di-Na salt, dihydrate: [68448-39-5].
Synth. by adding excess EtOH to an aq. soln. containing Mn(*II*) salt and disodium adenosine triphosphate (1:1). Light pink solid. μ_{eff} = 6.33μ_B. Loses $2H_2O$ at 75°, anhydrous complex stable in the temp. range 140-265°.
Di-Na salt, tetrahydrate: Synth. by dissolving dihydrate in H_2O followed by slow evaporation. Amorph. solid.

Bhattacharyya, R.G. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 733 (*synth, magnetism, ir*)
Mosset, A. *et al, Compt. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1980, **290**, 325 (*synth, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 33 (*rev, bibl*)

$C_{10}H_{12}MoN_5O_3^{\oplus}$ IC-006865

Bis(hydroxylamido)nitrosyl-2,2′-bipyridylmolybdenum(1+)
(2,2′-Bipyridine-N,N′)bis(hydroxylaminato-N,O) nitrosylmolybdenum(1+), 10CI



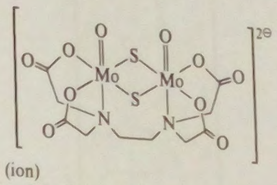
M 346.1 (ion)
Pentagonal bipyramidal at Mo.
Chloride: [70631-30-0].
Yellow cryst. Ir $\nu_{N=O}$ 1615 cm^{-1}.

Wieghardt, K. *et al, Angew. Chem., Int. Ed. Engl.*, 1979, **18**, 548 (*cryst struct, synth, ir*)
Wieghardt, K. *et al, Chem. Ber.*, 1980, **113**, 629 (*synth*)

$C_{10}H_{12}Mo_2N_2O_{10}S_2^{2\ominus}$ IC-006866

[μ-[[*N,N′*-1,2-Ethanediylbis[*N*-(carboxymethyl)glycinato](4−)-*O,O,O*^{N}:*N′,O′,O*^{N}]]dioxodi-μ-thioxodimolybdate(*V*)(2−), 9CI
μ-[Ethylenediaminetetraacetato]-di-μ-sulfidobis[oxomolybdate(V)](2−). Bis(μ-sulfido)(ethylenediaminetetraacetato)bis[oxomolybdate(V)]

[98652-24-5]



M 576.2 (ion)
Short Mo—Mo distance 280 pm indicating possible M—M bonding, diamagnetic. Pulse radiolysis in aq. soln. yields mixed valence ion $[Mo^{IV}Mo^{V}O_2S_2(EDTA)]^{3\ominus}$.
Di-Na salt: [62569-65-7].
Synth. by treatment of a soln. of $Na_2MoO_4.2H_2O$ saturated with H_2S, in H_2O, with $Na_3H_2EDTA.2H_2O$. Red-orange cryst $+2H_2O$ (H_2O). Diamagnetic.
Di-Cs salt: [42554-82-5].
Synth. by treatment of $Cs_4[(MoO_3)_2(EDTA)]$with H_2S. Red-orange cryst. $+2H_2O$ (H_2O). Diamagnetic.

[84785-89-7, 98652-26-7]

Spivak, B. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1173 (*cryst struct, deriv*)
Spivak, B. *et al, J. Less-Common Met.*, 1974, **36**, 249 (*cryst struct, deriv*)
Ott, V.R. *et al, Inorg. Chem.*, 1977, **16**, 2538 (*deriv, ir, uv, aq. electrochem*)
Kobayashi, H. *et al, Bull. Chem. Soc. Jpn.*, 1983, **56**, 108 (*deriv, esr, magnetism, struct*)
Rush, J.D. *et al, Inorg. Chem.*, 1985, **24**, 3895 (*synth, pulse radiolysis*)

$C_{10}H_{12}N_2Na_4O_8$ IC-006867

Tetrasodium ethylenediaminetetraacetate
(Ethylenedinitrilo)tetraacetic acid, tetrasodium salt, 8CI. Sodium edetate. Ethylenediaminetetraacetic acid, tetrasodium salt. [N,N′-1,2-Ethanediylbis(N-carboxymethyl) glycine] *tetrasodium salt, 9CI*

[64-02-8]

$(NaOOCCH_2)_2NCH_2CH_2N(CH_2COONa)_2$

M 380.1
Used widely in electroplating processes.
▷ AH5075000.
Dihydrate: [10378-23-1].
$C_{10}H_{16}N_2Na_4O_{10}$ M 416.2
Commercially available.
▷ Irritant.

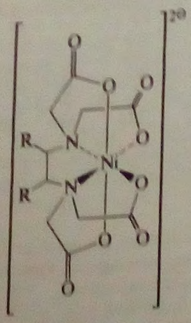
Nagai, T. *et al, Tenside Deterg.*, 1972, **9**, 317; *CA*, 1973, **78**, 45406 (*pmr*)
Baisden, P.A. *et al, Inorg. Chem.*, 1977, **16**, 1367 (*pmr*)
Nuttall, R.H. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1884 (*raman*)
Polyakova, I.A. *et al, Izv. Timiryazevsk. Skh. Akad.*, 1979, 167; *CA*, **91**, 174326 (*ir*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1607D (*haz, dihydrate*)

$C_{10}H_{12}N_2NiO_8^{2\ominus}$ IC-006868

(Ethylenediaminetetraacetato)nickelate(*II*)(2−)

*[(Ethylenedinitrilo)tetraacetato]nickelate(*II*)(2−), 8CI.* *[*N,N′-1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](6−)]-*nickelate*(II)(2−), 9CI*

[14931-84-1]



R = H

M 346.9 (ion)

Octahedral with rare hexadentate EDTA: steric restrictions usually allow H_2O coordination. Used in volumetric analysis of Ni. Many derivs. with partly protonated ligand also known. Salts with $[M(OH_2)_n]^{2\oplus}$ ions are one-dimensional ferrimagnets.

Na salt: [15708-55-1].
$C_{10}H_{12}N_2Na_2NiO_8$ M 392.8
Used for mercaptan oxidation and electroless plating.

Ca salt: [73729-48-3].
$C_{10}H_{20}CaN_2NiO_{12}$ M 459.0
Cryst. + $4H_2O$.

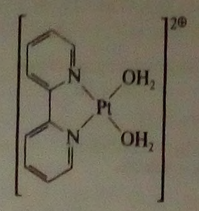
Tetraaquamanganese(2+) salt, dihydrate: [62227-88-7].
$C_{10}H_{24}MnN_2NiO_{14}$ M 509.9

Erickson, L.E. *et al, Inorg. Chem.*, 1971, **10**, 441 (*pmr*)
Solans, X., *Acta Crystallogr., Sect. C*, 1983, **39**, 435 (*cryst struct*)
Nesterova, Y.M. *et al, Koord. Khim.*, 1984, **10**, 129 (*cryst struct*)
Drillon, M. *et al, J. Magn. Magn. Mater.*, 1986, **54-57**, 1507 (*magnetism*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 219 (*rev*)

$C_{10}H_{12}N_2O_2Pt^{2\oplus}$ IC-006869

Diaqua(2,2′-bipyridine-*N,N′*)platinum(*II*)(2+), 9CI

Diaqua(2,2′-bipyridyl)platinum(II). *Diaqua(2,2′-dipyridyl)platinum*(II)



M 387.2 (ion)

Little-studied apart from synth. Suggested use of uv-vis and cd spectra of $Pt(bipy)^{2\oplus}$ moiety to monitor conformational changes in bifunctional substrates.

Nitrate: [64800-95-9].
Synth. from $AgNO_3$ + (2,2′-Bipyridine-*N,N′*) dichloroplatinum, IC-006724. Yellowish powder.

Perchlorate: [54822-53-6].
Synth. from $HClO_4$ + $[Pt(bipy)(OH)_2]$. Yellow solid.
▷ Potentially explosive.

Bielli, E. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 2133 (*synth*)
Chao, Y.Y.H. *et al, J. Am. Chem. Soc.*, 1977, **99**, 8024 (*synth, uv, cd*)

$C_{10}H_{12}N_2O_4Ru$ IC-006870

Dihydroxydioxobis(pyridine)ruthenium(*VI*), 9CI

Bis(hydroxo)dioxobis(pyridine)ruthenium(VI)

[38890-36-7]

As Dichlorodioxobis(pyridine)ruthenium(*VI*), IC-006798 with

X = OH

M 325.2

Octahedral. Monomeric in C_6H_6. A reformulation of the species originally reported as $RuO_4(Py)_2$. Prepd. by the reaction of RuO_4 with Py in CCl_4. Dark green diamagnetic solid. Ir ν_{RuO_2} 790 cm^{-1}, Raman ν_{RuO_2} 850 cm^{-1}.

Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1972, 1449 (*synth, ir*)
D'yachenko, Yu.I., *Sovrem Probl. Khim.*, 1973, 17 (*synth*)

$C_{10}H_{12}N_2O_8Sn_2$ IC-006871

μ-(Ethanediaminetetraacetato)ditin

μ-[(Ethylenedinitrilo)tetraacetato]ditin, 8CI. *μ-[*N,N′-1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinato*(4−)]]*ditin, 9CI.*
Distannous ethylenediaminetetraacetate

$[(OOCCH_2)_2NCH_2CH_2N(CH_2COO)_2]Sn_2$

M 525.6

Obt. as dihydrate.

Dihydrate: [12245-00-0].
$C_{10}H_{16}N_2O_{10}Sn_2$ M 561.6
Formed from $SnCl_2$ + EDTA in H_2O. Colourless prismatic tablets (H_2O). Spar. sol. H_2O. Struct. may be represented $Sn^{II}[Sn^{II}(EDTA).H_2O].H_2O$. One Sn is pseudo pentagonal bipyramidally coord. by EDTA with lone pair occupying an equatorial position. The second Sn is bonded to lone pairs on O of EDTA and may be regarded as 8-coord.

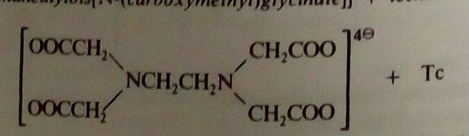
[34090-63-6]

Langer, H.C. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 767; 1967, **29**, 495 (*synth, ir*)
Van Remoortere, F.P. *et al, Inorg. Chem.*, 1971, **10**, 1511 (*cryst struct*)
McConnell, A.A. *et al, Spectrochim. Acta, Part A*, 1977, **33**, 459 (*ir, raman*)

$[C_{10}H_{12}N_2O_8Tc^{4\ominus}]$ IC-006872

Ethylenediaminetetraacetate technetium complex

*Ethane-1,2-diamine-*N,N,N′,N′*-tetraacetate + technetium.*
*1,2-Diaminoethane-*N,N,N′,N′*-tetraacetate + technetium.*
EDTA-technetium. Technetium-EDTA. [*N,N′-1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinate*]] + *technetium*



A range of ill-characterised complexes have been obtained by redn. of $TcO_4^{\ominus}$ in the presence of EDTA; a di-μ-oxo-ditechnetium(*IV*) and an oxotechnetate(*V*) species have been characterised and a Tc(*III*) complex obt. from Hexakis(thiourea-*S*)technetium(*III*)(3+), IC-005536.

Russell, C.D. *et al, Int. J. Appl. Radiat. Isot.*, 1978, **29**, 109 (*electrochem*)

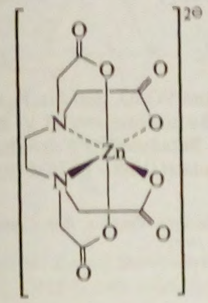
Russell, C.D. *et al, J. Nucl. Med.*, 1980, **21**, 354 (*characterisation*)
Bürgi, H.B. *et al, Inorg. Chem.*, 1981, **20**, 3829 (*cryst struct, dimer*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, Suppl. Vol. 2, 1983, 221 (*rev, bibl*)
Garcia Domenech, R., *Appl. Radiat. Isot.*, 1989, **40**, 536 (*biol*)
Hashimoto, M. *et al, J. Radioanal. Nucl. Chem.*, 1991, **153**, 283 (*synth*)

$C_{10}H_{12}N_2O_8Zn^{2\ominus}$ IC-006873

(Ethylenediaminetetraacetato)zincate(2−)

[(Ethylenedinitrilo)tetraacetato]zincate(2−), 8CI. *[[*N,N′-1,2-Ethanediylbis*[N-(*carboxymethylglycinato*)]](4−)]-*N,N′,O,O′,O^N,O^N′]zincate(2−), 9CI*

[12519-36-7]



M 353.6 (ion)

Octahedral at Zn. Rapid exchange occurs in soln. involving penta- to hexa-coordination.
Nutrient/fertiliser; used in photography; bleach-fixing solns.

Tetraaquamagnesium(2+) salt, dihydrate: [62313-89-7].
Magnesium zinc ethylenediaminetetraacetate hexahydrate
$C_{10}H_{24}MgN_2O_{14}Zn$ M 486.0
Octahedral Mg is coordinated to O from $4H_2O$ and to 2 from carbonyl oxygens of 2 adjacent EDTA groups; $2H_2O$ are water of crystallisation. Cryst.

Tetraaquamanganese(2+) salt, dihydrate: [63533-41-5].
Manganese zinc ethylenediaminetetraacetate hexahydrate
$C_{10}H_{24}MnN_2O_{14}Zn$ M 516.6
Cryst.

Tetraaquazinc(2+) salt, dihydrate: [12785-81-8]. *Dizinc ethylenediaminetetraacetate hexahydrate.*
Hexaaqua[*N,N′-1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](4−)*dizinc*
$C_{10}H_{24}N_2O_{14}Zn_2$ M 527.0
Two zinc environments: Zn(1) coordinated to the 2 N atoms and 4 × carbonyl oxygens. Zn(2) coordinated to O of $4H_2O$ and 2 from 2 adjacent EDTA groups. Two H_2O are water of crystallisation. Cryst.

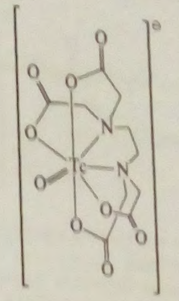
[14025-21-9, 14852-72-3, 37336-76-8, 37979-89-8, 51159-40-1, 53762-08-6, 64280-09-7, 71936-62-4]

Kula, R.J. *et al, J. Am. Chem. Soc.*, 1963, **85**, 2930 (*pmr*)
Anderegg, G., *Helv. Chim. Acta*, 1964, **47**, 1801 (*stability const*)
Pozhidaev, A.I. *et al, J. Struct. Chem. USSR* (*Engl. Transl.*), 1972, **13**, 690; 1973, **14**, 527 (*cryst struct*)
Yoshida, T. *et al, Bull. Chem. Soc. Jpn.*, 1974, **47**, 50 (*pe*)
Howarth, O.W. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 2271 (*cmr*)
Nuttall, R.H. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 39 (*thermal anal*)
Funaki, H.S. *et al, J. Am. Chem. Soc.*, 1982, **104**, 5325 (*stability const*)
Solans, X. *et al, Acta Crystallogr., Sect. C*, 1983, **39**, 435 (*cryst struct*)
Escriva, E. *et al, Transition Met. Chem.*, 1984, **9**, 184 (*ir*)
Isa, K., *CA*, 1986, **105**, 235035 (*ms*)
Escriva, E. *et al, Thermochim. Acta*, 1986, **104**, 223 (*thermal anal*)

$C_{10}H_{12}N_2O_9Tc^{\ominus}$ IC-006874

(Ethylenediaminetetraacetato)oxotechnetate(*V*)(1−)

*[[*N,N′-1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](4−)-*N,N′,O,O′]oxotechnetate(1−)*



M 403.1 (ion)

Pentagonal bipyramidal. Tc(*IV*) analogue may exist.
Synth. from $TcOCl_4^{\ominus}$ and H_4edta in anhydrous DMSO.

Ba salt (2:1): Cryst. Carboxylate O bridges Tc and Ba.

[86019-16-1]

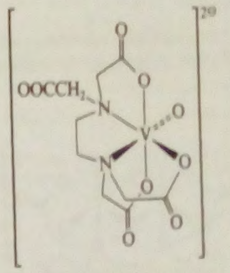
Bandoli, G. *et al, Coord. Chem. Rev.*, 1982, **44**, 191 (*cryst struct*)
Noll, B. *et al, Int. J. Appl. Radiat. Isot.*, 1983, **34**, 581 (*synth, uv, ir, magnetism*)

$C_{10}H_{12}N_2O_9V^{2\ominus}$ IC-006875

(Ethylenediaminetetraacetato)oxovanadate(*IV*)(2−)

*[[*N,N′-1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](4−)-*N,N′,O,O′,O″]oxovanadate*(IV)(2−), *11CI*

[12276-03-8]



M 355.1 (ion)

H-compd., Na salt: [19696-44-7].
Synth. from $VO(acac)_2$ and H_4EDTA in aq. $NaClO_4/HClO_4$ soln. Pale blue solid (H_2O).

Ba salt: [65531-64-8].
Pale blue cryst. + $6H_2O$.

[20648-98-0]

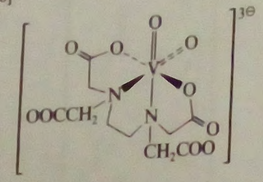
Nesterov, Ya.M. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1977, **237**, 350; *CA*, **88**, 57208v (*cryst struct, Ba salt*)
Sasaki, Y. *et al, Inorg. Chem.*, 1985, **24**, 772 (*synth, electrochem*)

$C_{10}H_{12}N_2O_{10}V^{3\ominus}$ IC-006876

Dioxo(ethylenediaminetetraacetato)vanadate(*V*)(3−)

[[N,N′-1,2-Ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N′,O,O′]dioxovanadate(V)(3−), 11CI

[68907-94-8]



M 371.1 (ion)

Octahedral anion with *cis*-dioxo groups.

Tri-Na salt: [34777-55-4].
Synth. by dissolving NH_4VO_3 in NaOH and crystallising from a soln. at pH 5 containing EDTA. White solid + $4H_2O$. Tri-K and tri-NH_4 salts also known.

Di-H deriv., NH_4 salt: [34777-57-6]. *Dioxo(dihydrogen ethylenediaminetetraacetato)vanadate(V) ammonium salt.*
[Dihydrogen(ethylenedinitrilo)tetraacetato-N,N′,O,O′] dioxovanadate(1−) ammonium salt, 8CI
Synth. from NH_4VO_3 + EDTA in H_2O at pH 2. Cryst. + $3H_2O$.

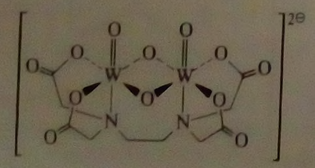
[38780-28-8]

Przyborowski, L. *et al, Helv. Chim. Acta*, 1965, **48**, 1556 (*synth, derivs*)
Scheidt, W.R. *et al, J. Am. Chem. Soc.*, 1971, **93**, 3873 (*cryst struct, di-H deriv*)
Hoard, J. *et al, J. Am. Chem. Soc.*, 1971, **93**, 3878 (*cryst struct, tri-Na salt*)

$C_{10}H_{12}N_2O_{12}W_2^{2\ominus}$ IC-006877

[μ-[[*N,N′*-1,2-Ethanediylbis[*N*-(carboxymethyl)glycinato]] (4−)-$N,O,O^N:N',O',N'$]]di-μ-oxodioxoditungstate(*V*) (2−), 10CI

[75521-40-3]



M 719.9 (ion)

Diamagnetism of salts can be explained by antiferromagnetic exchange through bridging oxygens or directly through a W—W bond; distorted octahedral coord. to W.

Di-K salt: [54275-52-4].
Obt. by metathesis of Ba salt with K_2SO_4. Air stable orange-red cryst. + $2H_2O$ (aq. EtOH), dec. at *ca.* 300°. Mod. sol. H_2O.

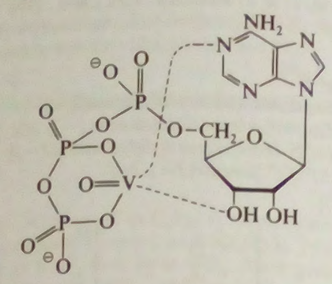
Ba salt: [54275-54-6].
Synth. from $K_2[WO_2(C_2O_4)_2].3H_2O$, EDTA, NaOAc, $CaCl_2$ and $BaCl_2$. Air stable orange-red cryst. + 3-$5H_2O$, dec. at *ca.* 300°. Sol. hot H_2O.

Novak, J. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 1061 (*synth, ir, uv, props, Ba, Na, K, NH_4 salts*)
Khalil, S. *et al, Inorg. Chim. Acta*, 1977, **25**, L83 (*cryst struct, Ba salt, uv*)
Khalil, S. *et al, Acta Crystallogr., Sect. B*, 1978, **34**, 3751 (*cryst struct, Ba salt*)

$C_{10}H_{12}N_5O_{14}P_3V^{2\ominus}$ IC-006878

[Adenosine-5′-(triphosphato)(4−)-$N^3,O^{P'},O^{P^-},O^3$] oxovanadate(*IV*)(2−), 11CI

[84605-49-2]



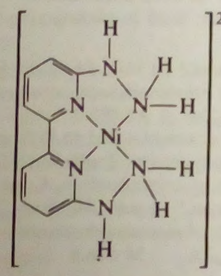
M 570.0 (ion)

Synth. in soln. from $VOSO_4$ and Na_2H_2ATP at acid pH. Of interest in the biochemistry of V. Blue soln. in H_2O. Closely related Bis[adenosine-5′-(triphosphato)(5−)-O^2,O^3]oxovanadate(*IV*)(8−), IC-010526 is formed at alkaline pH.

Sakurai, H. *et al. Biochem. Biophys. Res. Commun.*, 1982, **108**, 474 (*synth, P-31 nmr, cmr*)

$C_{10}H_{12}N_6Ni^{2\oplus}$ IC-006879

([2,2′-Bipyridine]-6,6′(1*H*′,1*H*′)-dionedihydrazone) nickel(*II*)(2+), 10CI



M 274.9 (ion)

Undergoes condensations with various aldehydes and ketones to afford macrocyclic complexes.

Diperchlorate: [53346-21-7].
Yellow cryst. (H_2O). Diamagnetic.
▷ Detonates violently on heating.

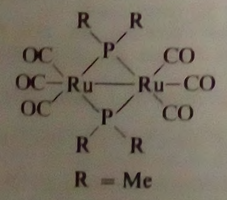
Lewis, J. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 734; 1978, 440 (*synth, reactions*)

$C_{10}H_{12}O_6P_2Ru_2$ IC-006880

Hexacarbonylbis[μ-(dimethylphosphino)]diruthenium, 9CI

Bis-μ-(dimethylphosphino)bis(tricarbonylruthenium)(I)

[36568-57-7]



R = Me

M 492.2

Synth. from P_2Me_4 + $Ru_3(CO)_{12}$ in C_6H_6 at 80-90°. Orange cryst. (C_6H_6/hexane). Sol. C_6H_6. Subl. *in vacuo*. Ir ν_{CO} 2069, 2038, 2033, 2001, 1989, 1979 cm^{-1}.

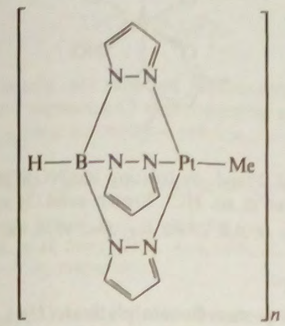
Candlin, J.P. *et al, Chem. Ind. (London)*, 1966, 1960 (*synth, ir*)
Dessy, R.E. *et al, J. Am. Chem. Soc.*, 1972, **94**, 746 (*synth, pmr, props*)

$C_{10}H_{13}BN_6Pt$ IC-006881

Methyl[tris(pyrazolyl)borato]platinum(*II*)

[Hydrotris(1H-pyrazolato-N^1)borato(1−)-N^2,N^2] methylplatinum(II), 9CI

[39395-33-0]



M 423.1

Probably polymeric. Forms monomeric complexes with eg. $F_3CC{\equiv}CCF_3$. Grey-brown solid. Sol. CH_2Cl_2. Mp >150°.

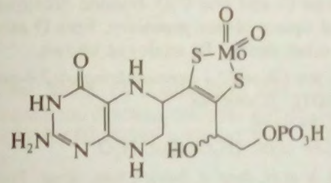
Clark, H.C. *et al, Inorg. Chem.*, 1974, **13**, 1291 (*synth, reactions*)

$C_{10}H_{13}MoN_5O_8PS_2$ IC-006882

Molybdenum cofactor

Molybdoenzyme molybdenum cofactor, 9CI. Molybdopterin. Moco

[73508-07-3]



Proposed structure

M 522.2

Molybdenum cofactor functions as a prosthetic metal in the 12 or so Mo-containing enzymes discovered, except nitrogenase which has its own Fe—Mo cofactor. Extremely unstable in free form.

Molybdenum and Molybdenum-Containing Enzymes, Coughlan, M.P., Ed., Pergamon, N.Y., 1980 (*book*)
Burgmayer, S.J.N. *et al, J. Chem. Educ.*, 1985, **62**, 943 (*rev*)
Metal Ions in Biology, Vol. 7: Molybdenum Enzymes, (Ed. Spiro, T.G.), John Wiley, N.Y., 1985 (*book*)
Taylor, E.C. *et al, J. Org. Chem.*, 1988, **53**, 5839 (*synth, bibl*)
Taylor, E.C. *et al, J. Am. Chem. Soc.*, 1989, **111**, 285 (*synth, bibl*)
Larsen, L. *et al, J. Chem. Soc., Perkin Trans. 1*, 1989, 2311, 2317 (*synth, bibl*)

$C_{10}H_{13}N_2NiO_8^{\ominus}$ IC-006883

[Ethylenediamine(monoacetic acid)triacetato]nickelate(*II*) (1−)

Ethylenedinitrilo(tetraacetato)nickelate(2−) hydrogen, 8CI

$Ni[HO_2CCH_2(OOCCH_2)NCH_2CH_2N(CH_2COO)_2]^{\ominus}$

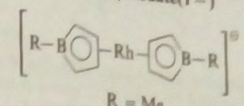
M 347.9 (ion)

Na salt, dihydrate: [20293-16-7].
$C_{10}H_{17}N_2NaNiO_{10}$ M 406.9
Pale lilac cryst.

Potopova, N.P. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 99 (*synth, ir*)

$C_{10}H_{14}B_2Rh^{\ominus}$ IC-006884

Bis(η⁵-1-methyl-1*H*-borole)rhodate(1−)



R = Me

M 258.7 (ion)

Me_4N salt: [110726-02-8].
Light yellow air-stable cryst. (Me_2CO/Et_2O). V. sol. Me_2CO, sol. H_2O. Mp 293-294°.

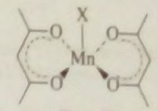
Herberich, G.E. *et al, J. Organomet. Chem.*, 1986, **312**, 13 (*synth, pmr, B-11 nmr*)

$C_{10}H_{14}BrMnO_4$ IC-006885

Bromobis(2,4-pentanedionato-*O,O′*)manganese(*III*), 9CI

Bromobis(acetylacetonato)manganese(III)

[51371-60-9]



X = Br

M 333.0

Square pyramidal struct. presumed. Synth. from $Mn(acac)_3$ and HBr in CH_2Cl_2. Hygroscopic green cryst. ($CHCl_3$/heptane). Sol. CH_2Cl_2, MeCN. Mp 158° dec. High spin Mn(*III*), monomeric in CH_2Cl_2. Solvolysed in H_2O and MeOH to give $Mn(acac)_2(solvent)_2^{\oplus}$.

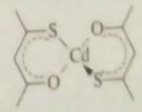
Isobe, K. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 250 (*synth, ir, uv, magnetism*)
Stutts, B.R. *et al, Inorg. Chem.*, 1975, **14**, 722 (*synth, ms, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 101 (*rev, bibl*)

$C_{10}H_{14}CdO_2S_2$ IC-006886

Bis(4-thioxo-2-pentanonato-*O,S*)cadmium, 9CI

Bis(2-thio-2,4-pentanedionato)cadmium
Bis(monothioacetylacetonato)cadmium

[16775-06-7]



M 342.7

Tetrahedral. Pale yellow needles (Me_2CO). Mp 159-161°.

Chaston, S.S.H. *et al, Aust. J. Chem.*, 1967, **20**, 1065 (*synth, ir*)
Siimann, O. *et al, J. Chem. Phys.*, 1971, **54**, 734.
Siimann, O. *et al, J. Am. Chem. Soc.*, 1974, **96**, 2353 (*synth, ir*)

$C_{10}H_{14}CdO_4$ IC-006887

Bis(2,4-pentanedionato-*O,O'*)cadmium

Bis(acetylacetonato)cadmium. Cadmium acetylacetonate

[14689-43-3]

M 310.6

The struct. contains infinite parallel chains of octahedral Cd atoms bridged by pairs of O atoms from 2 independent ligands. Prepd. from CdO + 2,4-pentanedione. White solid or reddish cryst. (EtOH). Mp 233°

[23880-59-0]

Read, M.J. *et al, J. Phys. Chem.*, 1955, **59**, 80 (*gaseous const*)
Hassanein, M. *et al, Z. Anorg. Allg. Chem.*, 1970, **373**, 80 (*synth, ir, nmr*)
Masden, E.N. *et al, J. Chem. Soc., Dalton Trans.*, 1975, 400 (*cryst struct*)
Schilderson, S.M., *J. Phys. Chem.*, 1976, **80**, 2834 (*use*)
Wilkie, C.A. *et al, J. Inorg. Nucl. Chem.*, 1978, **40**, 193 (*use*)
Memmit, P.G. *et al, J. Phys. Chem.*, 1981, **85**, 2087 (*C-113 nmr*)
Bueno, L. *et al, Can. J. Chem.*, 1983, **61**, 2141 (*synth, pmr*)

$C_{10}H_{15}ClMnO_4$ IC-006888

Chlorobis(2,4-pentanedionato-*O,O'*)manganese(*III*), 11Cl

Bis(acetylacetonato)chloromanganese(III)

[14690-80-3]

$Mn(acac)_2Cl$

M 288.6

Struct. not known. Synth. from $Mn(SCN)(acac)_2$, $AgClO_4$ and KCl. Brown cryst. ($CHCl_3$/heptane). Sol. CH_2Cl_2, MeCN. Mp 160° dec. Forms solvated species $[Mn(acac)_2L_2]^{\oplus}$ (L = H_2O or MeOH) in H_2O or MeOH. Reacts with HCl at −78° in CH_2Cl_2 to give $[MnCl_2(acac)(H_2O)]$.

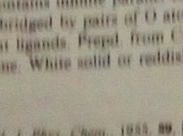
Isobe, K. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 250 (*synth, magnetism*)
Stutts, B.B. *et al, Inorg. Chem.*, 1975, **14**, 722 (*synth, props, ir, ms, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 101 (*rev, bibl*)

$C_{10}H_{14}ClNORuS_4$ IC-006889

Chloro(nitrosyl)bis(2,4-pentanedithionato-*S,S'*)ruthenium

Chlorobis(dithioacetylacetonato)(nitrosyl)ruthenium

[34032-01-4]



M 429.0

trans-Octahedral. Prepared by treating Diaquatrichloro(nitrosyl)ruthenium, IC-016865 in H_2O with pentane-2,4-dione and H_2S. Red cryst. Sol. H_2O, Me_2CO. Ir ν_{NO} 1840; $\nu_{Ru(Cl)}$ 300 cm^{-1}

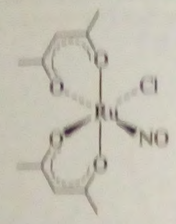
Heath, G.A. *et al, Aust. J. Chem.*, 1976, **23**, 2297 (*synth, ir, ms, uv, electrochem*)
Martin, R.L. *et al, Inorg. Chem.*, 1971, **10**, 2026 (*electrochem*)

$C_{10}H_{14}ClNO_2Ru$ IC-006890

Chloro(nitrosyl)bis(2,4-pentanedionato-*O,O'*)ruthenium, 9Cl

Bis(acetylacetonato)chloro(nitrosyl)ruthenium

[38171-57-3]



M 364.7

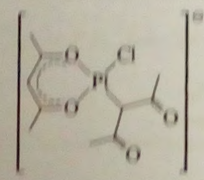
cis-Octahedral. Prepd. by treating $Ru(NO)(OH)_3$ with acetylacetone in aq. HCl. Brown solid. Ir ν_{NO} 1884 cm^{-1}.

Mukaida, M. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 1443 (*synth, ir*)

$C_{10}H_{14}ClO_4Pt^{\ominus}$ IC-006891

Chlorobis(2,4-pentanedionato)platinate(*II*)(1−)

(1-Acetylacetonyl)chloro(2,4-pentanedionato)platinate(1−), 8Cl. (1-Acetyl-2-oxopropyl)chloro(2,4-pentanedionato-O,O')platinate(1−), 9Cl. Bis(acetylacetonato)chloroplatinate(1−)



M 428.7 (ion)

Contains one *C*- and one *O,O'*-bonded diketonate to allow favoured square planar geometry. Free O atoms can chelate other metals. Br analogue known.

H compd.: see *Chloro(2,4-pentanedionato)(2,4-pentanedione) platinum*(II), *IC-006948*

K salt: [15258-91-0].

Pale yellow cryst. (H_2O). Sol. H_2O.

Grinberg, A.A. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1959, **4**, 137 (*synth, elec cond*)
Figgis, B.N. *et al, Nature (London)*, 1962, **195**, 1278 (*synth*)
Lewis, J. *et al, J. Chem. Soc.*, 1965, 6740 (*pmr*)
Gibson, D. *et al, J. Chem. Soc. A*, 1967, 72 (*synth, ir, pmr*)
Behnke, G.T. *et al, Inorg. Chem.*, 1968, **7**, 330 (*synth, ir*)
Mason, R. *et al, J. Chem. Soc. A*, 1969, 485 (*struct*)
Nakamura, Y. *et al, Inorg. Chem.*, 1975, **14**, 63 (*ir*)
Christian, D.F. *et al, Can. J. Chem.*, 1978, **56**, 2516 (*synth*)

$C_{10}H_{14}ClO_5V$ IC-006892

Chlorooxobis(2,4-pentanedionato-*O,O'*)vanadium(*V*), 11Cl

Bis(acetylacetonato)chlorooxovanadium(V)

[34606-63-8]

$VOCl(H_3CCOCHCOCH_3)_2$

M 300.6

Synth. from $VOCl_3$ + excess acac in boiling Et_2O; by hydrol. of $VCl_2(acac)_2$ in moist air; or by uv irradiation of $VO(OEt)(acac)_2$ in CCl_4. Has been used in catalysts for polym. of alkenes and elastomers. Dark blue solid.

Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1958, **296**, 36 (*synth from $VOCl_3$*)

Funk, H. *et al, Z. Anorg. Allg. Chem.*, 1959, **302**, 199 (*synth from VCl_3*)
Natta, G. *et al, Makromol. Chem.*, 1963, **69**, 163 (*use*)
U.S. Pat., 3 957 743, (1976); *C.A.*, **85**, 64435Bt (*use*)
Rehder, D., *Z. Naturforsch., B*, 1977, **32**, 771 (*V-51 nmr*)
Kuchmii, S.Ya. *et al, Ukr. Khim. Zh. (Russ. Ed.)*, 1980, **46**, 806; *C.A.*, **94**, 98098x (*photochem synth*)

$C_{10}H_{14}Cl_2CrN_2O_2$ IC-006893

Disquadichlorobispyridinechromium(*II*)

$CrCl_2(OH_2)_2(Py)_2$

M 317.1

Octahedral, config. not reported. Similar complexes known with Br or I replacing Cl and containing substituted pyridines. Green air-sensitive solid. μ_{eff} = 4.79μ_B (292K).

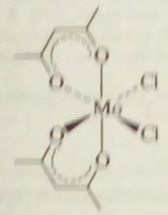
Earnshaw, A. *et al, Chem. Ind. (London)*, 1965, 1521 (*synth, magnetism*)
Beech, G. *et al, J. Chem. Soc. A*, 1969, 512 (*rgn*)
Khamar, M.M. *et al, Inorg. Chim. Acta*, 1978, **28**, 245; 1979, **36**, 223 (*synth, vis, ir, magnetism*)

$C_{10}H_{14}Cl_2MoO_4$ IC-006894

Dichlorobis(2,4-pentanedionato-*O,O'*)molybdenum(*IV*), 9Cl

Bis(acetylacetonato)dichloromolybdenum(IV)

[36470-64-1]



M 365.0

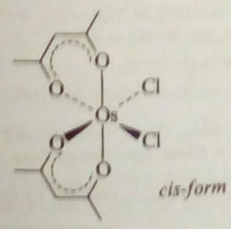
cis-Octahedral. Synth. by treatment of $MoCl_4$.2MeCN with 2,4-pentanedione. Starting material. Cryst. (Me_2CO). Sol. MeCN, EtOH, DMF with dec. μ_{eff} = 2.63μ_B (296.3K).

van den Bergen, A. *et al, Aust. J. Chem.*, 1972, **25**, 705 (*synth, ir, magnetism, uv-vis*)
Chen, G.J.J. *et al, Inorg. Chim. Acta*, 1979, **35**, 93 (*use*)
Kan, C.-T., *J. Chem. Soc., Dalton Trans.*, 1982, 2309 (*use*)

$C_{10}H_{14}Cl_2O_4Os$ IC-006895

Dichlorobis(pentane-2,4-dionato-*O,O'*)osmium(*IV*), 10Cl

Bis(acetylacetonato)dichloroosmium(IV)



cis-form

M 459.3

Synth. from $K_2[OsCl_6]$ and 1:1 mixt. of 2,4-pentanedione + H_2O. Isomers separated by chromatog. on silica gel. Sol. hexane.

cis-form [70366-29-9]

Dark solid.

trans-form [70398-27-5]

Red microcryst. Spar. sol. CH_2Cl_2. Mp 268-270° dec. μ_{eff} = 1.29μ_B

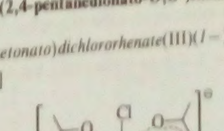
Preetz, W. *et al, Z. Naturforsch., B*, 1979, **34**, 593 (*uv, ir, raman, synth*)
Behling, T. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2109 (*synth, ir, ms, uv*)

$C_{10}H_{14}Cl_2O_4Pd_2$ IC-006896

Di-μ-chlorobis(2,4-pentanedionato-*O,O'*)dipalladium(*II*), 10Cl

Bis(acetylacetonato)dichlorodipalladium

[65027-68-1]



R = CH_3, X = Cl

M 481.9

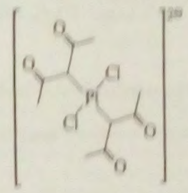
Slowly rearranges to isomer with Pd bonded to deprotonated CH_2 and C=C of enolised diketonate. Brown 'fuzzy' (?) solid.

Kanda, Z. *et al, Inorg. Chem.*, 1978, **17**, 910 (*synth, ir*)

$C_{10}H_{14}Cl_2O_4Pt^{IS}$ IC-006897

Dichlorobis(2,4-pentanedionato-*O,O'*)platinate(*II*)(2−)

Bis(1-acetylacetonyl)dichloroplatinate(2−), 8Cl



M 464.2 (ion)

Example of Pt favouring unusual *C*-coordination of diketonate, thereby facilitating favoured square planar geometry.

Di-Na salt, dihydrate: [15277-99-3].

Yellow solid. Sol. H_2O.

Di-K salt: Bright yellow cryst. Sol. H_2O.

[19356-42-4]

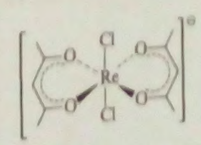
Behnke, G.T. *et al, Inorg. Chem.*, 1967, **6**, 433, 440 (*synth, ir*)

$C_{10}H_{14}Cl_2O_4Re^{\ominus}$ IC-006898

Dichlorobis(2,4-pentanedionato-*O,O'*)rhenate(*III*)(1−), 10Cl

Bis(acetylacetonato)dichlororhenate(III)(*1−*)

[70199-16-5]



M 455.3 (ion)

Na salt: [71078-20-1].

Green solid ($MeCN/Et_2O$). Sol. MeCN, H_2O.

K salt: [71078-21-2].
Synth. from $Re(acac)_2Cl_2$ and K shavings in MeCN. Green solid ($MeCN/Et_2O$). Sol. MeCN, H_2O.

Tl(I) salt: [71078-19-8].
Synth. from $Re(acac)_2Cl_2$ and Tl(acac) in Et_2O under reflux. Green solid.

Ph_4As salt: Synth. from the K salt and Ph_4AsCl in H_2O. Green cryst. ($MeCN/Et_2O$).

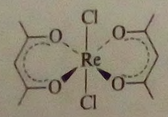
Lock, C.J.L. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 951 (*cryst struct*)
Lock, C.J.L. *et al, Can. J. Chem.*, 1979, **57**, 1252 (*synth, ir, uv*)

IC-006899

$C_{10}H_{14}Cl_2O_4Re$

Dichlorobis(2,4-pentanedionato-*O,O'*)rhenium(*IV*), 9Cl

Bis(acetylacetonato)dichlororhenium(IV)



trans-form

M 455.3
Octahedral.

cis-form [39039-00-4]
Minor isomer. Isol. from filtrate of *trans* preparation. Reddish-brown cryst.

trans-form [18907-37-4]
Monomeric. Synth. from $ReOCl_2(acac)(PPh_3)$ and acac. Other methods are also available. Orange cryst. (C_6H_6/CCl_4 or $CHCl_3$/pet. ether). Sol. $CHCl_3$. Mp 297-299° dec.

Courrier, W.D. *et al, Can. J. Chem.*, 1972, **50**, 1797 (*synth, uv, raman, ms, magnetism, props*)
Brown, I.D. *et al, Can. J. Chem.*, 1973, **51**, 2073 (*cryst struct*)

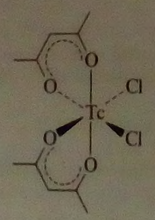
IC-006900

$C_{10}H_{14}Cl_2O_4Tc$

Dichlorobis(2,4-pentanedionato-*O,O'*)technetium(*IV*), 11Cl

Bis(acetylacetonato)dichlorotechnetium(IV)

[71128-07-9]



M 368.0
cis-Octahedral. Synth. from $TcCl_4(PPh_3)_2$ + pentanedione, or by refluxing $TcCl_6^{2\ominus}$ in pentanedione. Catalyst for dicyclopentadiene oxidation. Brown solid. Spar. sol. halogenated solvs.; insol. most org. solvs. Mp 240°.

Mazzi, U. *et al, Transition Met. Chem.*, 1979, **4**, 151 (*synth, ir, uv*)
Schnurpfeil, D. *et al, J. Prakt. Chem.*, 1983, **325**, 848 (*use*)

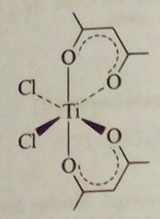
IC-006901

$C_{10}H_{14}Cl_2O_4Ti$

Dichlorobis(2,4-pentanedionato-*O,O'*)titanium(*IV*), 11Cl

Bis(acetylacetonato)dichlorotitanium(IV)

[17099-86-4]



cis-form

M 317.0
Manuf. from $TiCl_4$ in C_6H_6 with 2,4-pentanedione and CaO. Catalyst for olefin polym. Commercially available.

cis-form [16986-94-0]
Synth. from $TiCl_4$ and 2,4-pentanedione in CH_2Cl_2. Orange-red solid. Sol. CH_2Cl_2, $PhNO_2$, $CHCl_3$. Mp 191-192°.

trans-form [42532-19-4]
Probably only known in soln.

Serpone, N. *et al, Inorg. Chem.*, 1969, **8**, 2379 (*props*)
Ger. Pat., 1 495 259, (1973); *CA*, **79**, 19737g (*epoxy hardener, trans-form*)
Fay, R.C. *et al, Inorg. Chem.*, 1974, **13**, 1309 (*pmr*)
Brauer, G., *Handbuch Präp. Anorg. Chem.*, 3rd Ed., Ferdinand Enke Verlag, 1975-1981, **2**, 1391 (*synth*)
Tweedy, H.E. *et al, J. Mol. Catal.*, 1978, **3**, 239 (*use, trans-form*)
Inorg. Synth., 1979, **19**, 145 (*synth, cis-form*)
Smidtke, H.-H. *et al, Inorg. Chem.*, 1981, **20**, 2766 (*uv-vis, cis-form*)
Nedorezova, P.M. *et al, Vysokomol. Soedin., Ser. B*, 1986, **28**, 163; *CA*, **105**, 60978w (*use*)

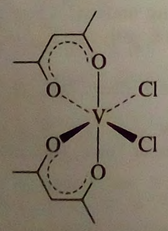
IC-006902

$C_{10}H_{14}Cl_2O_4V$

Dichlorobis(2,4-pentanedionato-*O,O'*)vanadium(*IV*), 11Cl

Bis(acetylacetonato)dichlorovanadium(IV)

[38991-25-2]



cis-form

M 320.0
Octahedral. Prob. exists as *cis/trans* mixt. Both isomers are synth. by reaction of $VO(acac)_2$ with $SOCl_2$ or PCl_5 in C_6H_6. Dark, air-sensitive solid.

[42532-52-5, 77340-91-1]

Van Dreel, R.B. *et al, J. Am. Chem. Soc.*, 1977, **94**, 7935 (*synth, ir*)
Pasquali, M. *et al, Inorg. Chem.*, 1979, **18**, 2401 (*synth*)
Jezierski, A. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1 (*synth, esr*)
Jezierski, A., *Inorg. Chim. Acta*, 1985, **98**, L1 (*synth, esr*)

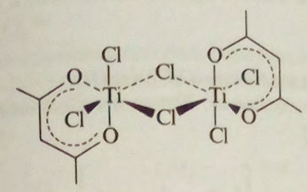
IC-006903

$C_{10}H_{14}Cl_6O_4Ti_2$

Di-μ-chlorotetrachlorobis(2,4-pentanedionato-*O,O'*)dititanium(*IV*), 10Cl

Di-μ-chlorobis[acetylacetonatodichlorotitanium(IV)]

[36482-44-7]



M 506.6
In solution a 5-coord. monomer is formed. Synth. e.g. from $TiCl_4$ and 2,4-pentanedione in C_6H_6. Dark red solid. Sol. CH_2Cl_2.

Monomer: (*Acetylacetonato*)*trichlorotitanium*(IV). *Trichloro*(*2,4-pentanedionato*-O,O')*titanium*(IV)
$C_5H_7Cl_3O_2Ti$ M 253.3

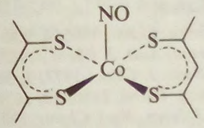
Serpone, N. *et al, J. Chem. Soc., Chem. Commun.*, 1972, 217 (*cryst struct, synth, ir, pmr*)
Serpone, N. *et al, Inorg. Chem.*, 1977, **16**, 2381, 2702.

IC-006904

$C_{10}H_{14}CoNOS_4$

Nitrosylbis(2,4-pentanedithionato-*S,S'*)cobalt(*I*), 9Cl

[50986-65-7]



M 351.4
Dark brown cryst. solid. Disproportionates in soln. to give $Co(NO)_2(C_5H_7S_2)$ and $Co(C_5H_7S_2)_3$.

Hendrickson, A.R. *et al, Inorg. Chem.*, 1974, **13**, 1279 (*synth, ir, pmr*)

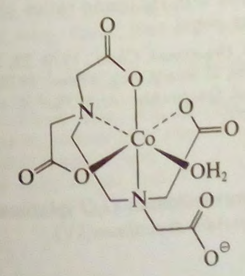
IC-006905

$C_{10}H_{14}CoN_2O_9^{\ominus}$

Aqua[ethylenediaminetetraacetato)cobaltate(*III*)(1−)

Aqua[[N,N'-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4*−)-N,N',O,O',O^N]*cobaltate*(*1*−), *11Cl, 10Cl*

[24340-68-9]



M 365.1 (ion)
EDTA acts as a quinquedentate ligand about octahedral Co. H_2O coordinates in the one remaining space.

Ba salt (2:1): [105992-74-3].
Synth. from $BaCl_2.2H_2O$, and $CoCl_2.6H_2O$ and $Na_2EDTA.2H_2O$. Cryst. + $6H_2O$.

H compd.: [14024-68-1].
$C_{10}H_{15}CoN_2O_9$ M 366.1
Red-violet needles + $3H_2O$. Spontaneously resolves.

[88200-20-8]

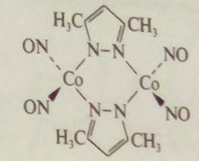
Dyke, R. *et al, J. Chem. Soc.*, 1960, 1998 (*soln kinetics*)
Okazaki, H. *et al, Inorg. Chim. Acta*, 1983, **74**, 169 (*cryst struct, H compd, cd*)
Zhou, K. *et al, Jiegou Huaxue*, 1985, **4**, 218; *CA*, **106**, 26071 (*cryst struct, Ba salt*)

IC-006906

$C_{10}H_{14}Co_2N_8O_4$

Bis[μ-(3,5-dimethyl-1*H*-pyrazolato-N^1,N^2)]tetranitrosyldicobalt, 10Cl

[72099-07-1]



M 428.1
Tetrahedral Co with bridging pyrazolato ligands. Black cryst. Sol. C_6H_6.

Chong, K.S. *et al, Can. J. Chem.*, 1979, **57**, 3119 (*synth, pmr, ms, cryst struct*)

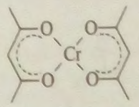
IC-006907

$C_{10}H_{14}CrO_4$

Bis(2,4-pentanedionato-*O,O'*)chromium(*II*), 9Cl, 8Cl

Bis(acetylacetonato)chromium(II). *Chromium*(II) *acetylacetonate. Chromous acetylacetonate*

[14024-50-1]



M 250.2
Planar; mean Cr—O 198 pm. Essentially planar, with weak interactions of metal (305 pm) with methine C atoms of ligands in adjacent molecules. Synth. from aq. slurry of $Cr(OAc)_2$ + 2 equivs. acetylacetone. Must be isol. rapidly and dried at 100° *in vacuo* for sev. hours. Reducing agent, useful in inner sphere redox reactions. Light yellow powder. Slowly oxidised by H_2O. Almost insol. H_2O; sl. sol. CS_2, EtOH. $Subl._{0.01}$ 100-105°. Dec. at 218-219°.

▷ Pyrophoric.

Inorg. Synth., 1966, **8**, 125 (*synth*)
Cotton, F.A. *et al, Inorg. Chim. Acta*, 1977, **24**, 231 (*cryst struct*)
Reed, C.A. *et al, Inorg. Chem.*, 1978, **17**, 2666 (*use*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 717, 738 (*rev*)

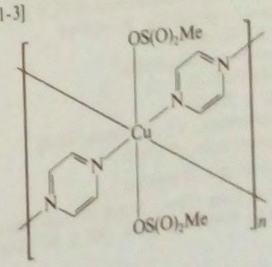
IC-006908

$C_{10}H_{14}CuN_4O_6S_2$

Bis(methanesulfonato-*O*)bis(pyrazine-N^4)copper(*II*)

poly-*Bis(pyrazine)bis(methanesulfonato*-O)*copper*(II)

[111287-41-3]



M 413.9
Struct. contains parallel sheets, each consisting of infinite square array of Cu(*II*) ions bridged by 2 types of bidentate pyrazine ligands. Tetragonally distorted octahedral geometry around Cu. Pale blue cryst. (MeOH). Insol. MeOH.

Haynes, J.S. *et al*, *Can. J. Chem.*, 1987, **65**, 420 (*synth, struct, ir, magnetism*)

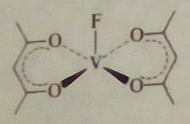
IC-006909

$C_{10}H_{14}FO_4V$

Fluorobis(2,4-pentanedionato-*O,O'*)vanadium(*III*), 11Cl

Bis(acetylacetonato)fluorovanadium(III)

[90461-85-1]



M 268.1
Square pyramidal. Synth. from $(N_2H_5)VOF_3$ and acac in H_2O. Blue-green solid. Sol. C_6H_6. Mp 246-248°. Paramagnetic, $\mu_{eff} = 2.77\mu_B$.

Chaudhuri, M.K. *et al*, *Inorg. Chem.*, 1984, **23**, 2367 (*synth, ir, magnetism, ms*)

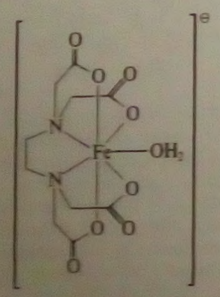
IC-006910

$C_{10}H_{14}FeN_2O_9^{\ominus}$

Aqua(ethylenediaminetetraacetato)ferrate(*III*)(1 −)

Aqua[N,N′-*1,2-ethanediylbis*[N-*carboxymethylglycinato*]]
(*4*)-N,N′,O,O′,O^N]*ferrate*(*1* −)

[36670-04-9]



M 362.0 (ion)
Seven coordinate Fe(*III*). Interacts with cytochrome C.
Na salt: [19413-44-6].
Yellow-brown cryst. + $2H_2O$.
K salt: [19496-00-5].
Brown cryst. + $1H_2O$. Various other alkali metal salts also known.
Ag(I) salt: [89997-28-4].
Yellow brown cryst. + $2H_2O$.
TI(I) salt: [90241-61-5].
Yellow brown cryst. + $1H_2O$.
H compd: see *Aquaethylenediamine-N,N,N′,N′-tetraacetate*(*3* −)-[*iron*(III), *IC-006936*
NH_4 salt: [103775-65-1].
Forms mono- and dihydrates.
Et_4N salt: [96411-25-5].
Red cryst. + $2H_2O$.
Ethylenediammonium(*1* +) *salt*: [96442-53-4].
Yellow-brown cryst. + $6H_2O$.

[19413-44-6, 21626-24-4, 28784-18-1]

Lind, M.D. *et al*, *Inorg. Chem.*, 1964, **3**, 34 (*cryst struct*)
Kennard, C.H.L., *Inorg. Chim. Acta*, 1967, **1**, 347 (*struct*)

Solans, X. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 635; 1985, **41**, 525 (*struct*)
Lopez-Alcala, J.M. *et al*, *Acta Crystallogr., Sect. C*, 1984, **40**, 939 (*struct*)
Takeda, M., *Hyperfine Interact.*, 1986, **28**, 737; *CA*, **105**, 90029e (*mössbauer*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **2**, 779 (*rev*)

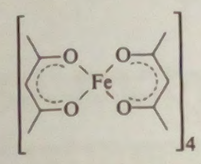
IC-006911

$C_{10}H_{14}FeO_4$

Bis(2,4-pentanedionato-*O,O'*)iron(*II*)

Iron(II) *acetylacetonate. Ferrous acetylacetonate*

[14024-17-0]



M 254.0
Tetrameric with distorted octahedral Fe. Catalyst. Toner and developer. Flame retardant.

Tetramer: [64578-39-8]. *Bis*[μ_3-(*1-acetyl-2-oxopropyl*-C^1:O^1:O^1:O^2)]*tetrakis*[μ-(*2,4-pentanedionato*-O:O,O′)]*bis*(*2,4-pentanedionato*-O,O′)*tetrairon*, *10Cl*.
Bis(acetylacetonato)iron tetramer
$C_{40}H_{56}Fe_4O_{16}$ M 1016.2
Synth. from $FeCl_2.4H_2O$ + HL. Orange-brown cryst. Spar. sol. C_6H_6, toluene. Subl. 85°. $\mu_{eff} = 5.4\mu_B$.
Dihydrate: [56143-49-8].

Fackler, J.P. *et al*, *Inorg. Chem.*, 1965, **4**, 920 (*magnetism*)
Buckingham, D.A. *et al*, *Aust. J. Chem.*, 1967, **20**, 281 (*synth*)
Cotton, F.A. *et al*, *Nouv. J. Chim.*, 1977, **1**, 301 (*cryst struct*)
Nicolini, C. *et al*, *Inorg. Chem.*, 1980, **19**, 2676 (*mössbauer*)
Moxon, N.T. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 491 (*magnetism*)

IC-006912

$C_{10}H_{14}HgO_4$

Bis(2,4-pentanedionato)mercury

Mercury acetylacetonate

[14024-55-6]

$[(H_3CCO)_2CH]_2Hg$

M 398.8
Hg is bound to the γ-carbon of the ligand and is not chelated through the O atoms. White solid. Hg acetylacetonates with Hg:ligand ratios of 1:1 and 2:3 have also been prepd.

Bonati, F. *et al*, *J. Organomet. Chem.*, 1970, **22**, 5 (*synth*)
Hassanein, M. *et al*, *Z. Anorg. Allg. Chem.*, 1970, **373**, 80 (*synth*)
Macklin, J.W. *et al*, *Spectrochim. Acta, Part A*, 1976, **32**, 1459 (*synth, ir, raman*)

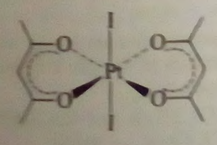
IC-006913

$C_{10}H_{14}I_2O_4Pt$

Diiodobis(2,4-pentanedionato-*O,O'*)platinum(*IV*), 9Cl

Bis(acetylacetonato)diiodoplatinum(IV)

[39899-64-4]



M 647.1

Octahedral struct. with *trans*-iodides unlike most $[MX_2(diket)_2]$. Synth. from $[Pt(acac)_2] + I_2$. Amber-coloured diamond-shaped plates; solns. in CCl_4 slowly dec. with loss of I_2. Sol. C_6H_6, CCl_4.

Cook, P.M. et al, J. Chem. Soc., Dalton Trans., 1973, 294 (*synth*)

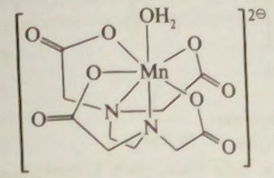
IC-006914

$C_{10}H_{14}MnN_2O_9^{2\ominus}$

Aqua(ethylenediaminetetraacetato)manganate(2 −)

Aqua[N,N′-*1,2-ethanediylbis*[(N-*carboxymethyl*)*glycinato*]]
(*4* −)-N,N′,O,O′,O^N]*manganate*(*2* −), *11Cl*

[38702-79-9]



M 361.1 (ion)
7-Coord. anions; geometry similar to $[NbF_7]^{\ominus}$. Used in detn. of Mn; removal of the radionuclide ^{54}Mn from mammalian bodies; extraction of $MnCO_3$ from rocks.

Hexaaquamagnesium(*2* +) *salt, dihydrate*: [96042-41-0].
Synth. from aq. suspensions of $Mg_2(edta).9H_2O$ and $Mn_2(edta).9H_2O$.

Tetraaquamanganese(*2* +) *salt, dihydrate*: Synth. from $MnCO_3$ and boiling aq. H_4edta at pH 6-7. Pale pink cryst. (H_2O). $[Mn(OH_2)_4]^{2\oplus}$ is attached to two O atoms of carboxylate groups in anion to give octahedral $Mn^{2\oplus}$. $\mu_{eff} = 5.87\mu_B$ (293K).

Di-H compd, trihydrate:
$C_{10}H_{22}MnN_2O_{12}$ M 417.2
Synth. from $MnCO_3$ and hot satd. aq. H_4edta. Air-stable cryst. (H_2O). $\mu_{eff} = 6.04\mu_B$ (293K). Reacts with $MHCO_3$ or M_2CO_3 to form the salts $M_2Mn(edta).nH_2O$; M = Li, Na, K, Rb.

H compd., Mn(II) *salt*, (*2:2:1*) *octahydrate*:
Manganese(*2* +) *bis*[(*hydrogen ethylenediaminetetraacetato*)*aquamanganate*(*1* −)] *octahydrate*
$C_{20}H_{46}Mn_3N_4O_{26}$ M 923.4
Synth. from $MnCO_3$ + warm dil. aq. H_4edta. Cryst. (H_2O). Formulated as $Mn[Mn(Hedta)(OH_2)]_2.8H_2O$.

Brentzinger, H. *et al*, *Z. Anorg. Allg. Chem.*, 1948, **256**, 65 (*synth*)
Skramovský, S. *et al*, *Collect. Czech. Chem. Commun.*, 1962, **27**, 1374 (*magnetism, synth, di-H compd*)
Richards, S. *et al*, *Inorg. Chem.*, 1964, **3**, 27 (*synth, cryst struct, Mn*(*II*) deriv)
Pozhidaev, A.I. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1972, **13**, 323 (*synth, cryst struct*)
Paulík, J. *et al*, *J. Therm. Anal.*, 1976, **10**, 123 (*dta*)
Pechurova, N.I. *et al*, *Moscow Univ. Chem. Bull.* (*Engl. Transl.*), 1978, **38**, 48 (*di-H compd, ir, tga*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 38, 41 (*rev, bibl*)

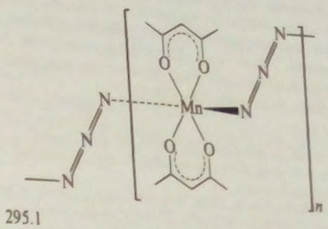
IC-006915

$C_{10}H_{14}MnN_3O_4$

Azidobis(2,4-pentanedionato-*O,O'*)manganese(*III*), 11Cl

Bis(acetylacetonato)azidomanganese(III)

[52242-28-1]



M 295.1
High spin manganese(*III*) complex. Prepared from $Mn(acac)_3$ and NaN_3 plus H_2SO_4. Brown air-stable cryst. (MeCN). Sol. common polar solvs. Mp 200° dec.

[52242-29-2]

Stults, B.R. *et al*, *Inorg. Chem.*, 1975, **14**, 722 (*synth, ir, ms, cryst struct, molar cond, magnetism*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 99 (*rev, bibl*)

IC-006916

$C_{10}H_{14}MnO_4$

Bis(2,4-pentanedionato-*O,O'*)manganese(*II*), 11Cl

Manganese(II) *acetylacetonate. Bis(acetylacetonato) manganese*(II)

[14024-58-9]

$Mn(acac)_2$

M 253.1
Struct. not known. Trimeric in non-coordinating solvs. Prepd. by dehydration of $Mn(acac)_2(OH_2)_2$ *in vacuo*. Polym. catalyst. Colourless cryst. Spar. sol. H_2O, sl. sol. MeOH, EtOH, Me_2CO. Subl. 90° *in vacuo*. Reacts with mono- or bidentate ligands e.g. amines or nitrogen heterocycles to give compds. of the type $Mn(acac)_2L_2$.

▷ OO9350000.

Trimer:
$C_{30}H_{42}Mn_3O_{12}$ M 759.4

Holm, R.H. *et al*, *J. Am. Chem. Soc.*, 1958, **80**, 5658 (*str*)
Inorg. Synth., 1960, **6**, 164 (*synth*)
Graddon, D.P. *et al*, *Aust. J. Chem.*, 1964, **17**, 1119 (*synth, magnetism*)
Nishikawa, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 155 (*ir*)
Kaeriyama, K., *Bull. Chem. Soc. Jpn.*, 1974, **47**, 753 (*props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 66 (*rev, bibl*)

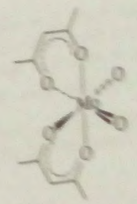
IC-006917

$C_{10}H_{14}MoO_6$

Dioxobis(2,4-pentanedionato-*O,O'*)molybdenum(*VI*), 9Cl

Bis(acetylacetonato)dioxomolybdenum(VI)
Molybdenylacetylacetonate. Bis(2,4-pentanedione) dioxomolybdenum(VI). *Molybdenum bis(acetylacetonate)*

[17524-05-9]



M 326.1
Distorted octahedral arrangement about Mo, with cis—MoO_2 groups. Synth. by treatment of $Na_2MoO_4.2H_2O$ in dil. HCl with acacH, with adjustment of pH. Commercially available. Starting material; catalyst for epoxidation of alkenes, polym. of vinyl compds., manuf. of polyurethanes, adhesives and sealants. Yellow cryst. (EtOH/2,4-pentanedione). V. stable if washed and dried. Slowly turns blue when exposed to sunlight. Mp 179° (175°).

[21884-95-7]

Jones, M.M. *J. Am. Chem. Soc.*, 1959, **81**, 3188 (*synth*)
Moore, F.W. *et al, Inorg. Chem.*, 1968, **7**, 2511 (*ir, pmr, uv, conductance, struct*)
Gehrke, H. *et al, Inorg. Chim. Acta*, 1969, **3**, 623 (*synth, ir, uv*)
Ger. Pat., 2 159 922, (1972); *CA*, **77**, 102921h (*use, catalyst*)
Sheldon, R.A. *et al, J. Catal.*, 1973, **31**, 427 (*use, catalyst*)
Krasochka, O.N. *et al, J. Struct. Chem. USSR (Engl. Transl.)*, 1975, **16**, 648 (*cryst struct*)
Pilcher, G. *et al, J. Chem. Soc., Dalton Trans.*, 1978, 1311 (*thermodyn*)
Guilloti, M. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 902 (*use*)
Japan. Pat., 81 86 909, (1981); *CA*, **95**, 170087n (*use, catalyst*)
Yamamoto, Y. *et al, Chem. Lett.*, 1986, 73 (*use, catalyst*)
Hinshaw, C.J. *et al, Inorg. Chem.*, 1989, **28**, 4483 (*use*)
Mohanty, R.N. *et al, Polyhedron*, 1990, **9**, 1011 (*use*)

$C_{10}H_{14}N_2Na_2O_8$ IC-006918

Ethylenediaminetetraacetic acid, disodium salt
Disodium ethylenediaminetetraacetate. N,N'-1,2-Ethanediylbis[N-carboxymethyl)glycine disodium salt, 9CI. (Ethylenedinitrilo)tetraacetic acid, disodium salt, 8CI

[139-33-3]

$NaOOCCH_2N(CH_2COOH)CH_2CH_2N(CH_2COOH)CH_2COONa$

M 336.2
Commercially available as 0.1*M* aq. soln. or as dihydrate. Volumetric standard for detn. of Mg^{2+}, Ca^{2+}

▶ AB4375000

Dihydrate: [6381-92-6]
$C_{10}H_{18}N_2Na_2O_{10}$ M 372.2
Commercially available.

Novák, A. *et al, Bull. Soc. Chim. Fr.*, 1965, 1440 (*ir*)
Stolyarov, K.P. *et al, CA*, 1967, **66**, 60467 (*uv-vis*)
Russell, R.H. *et al, J. Chem. Soc., Dalton Trans.*, 1977, 1884 (*raman*)
Djordjevic, C. *et al, J. Less-Common Met.*, 1983, **94**, 355 (*cmr, pmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1666D (*haz*)

$C_{10}H_{14}N_2O_8Sn$ IC-006919

Dihydrogen (ethylenediaminetetraacetato)stannate(*II*)
[Dihydrogen(ethylenedinitrilo)tetraacetato]tin, 8CI

[23314-34-3]

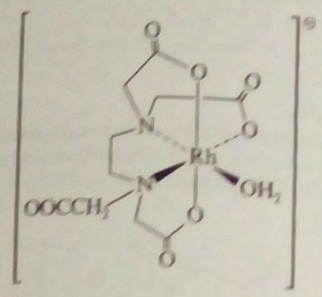
$[(HOOCCH_2)_2NCH_2CH_2N(CH_2COO)_2]Sn$

M 408.9
Struct. not elucidated. Synth. from solns. of $SnCl_2$ and Na_4(edta) at pH 1.5. White orthorhombic cryst. Sl. sol. H_2O (1.9%). Dec. in aq. soln. if exposed to O_2.

Langer, H.G. *et al, J. Inorg. Nucl. Chem.*, 1964, **26**, 767 (*ir, Na salt*)
Lebedeva, R.N. *et al, Zh. Neorg. Khim.*, 1967, **12**, 1093; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1967, **12**, 575 (*synth, ir*)

$C_{10}H_{14}N_2O_9Rh^{\ominus}$ IC-006920

Aqua(ethylenediaminetetraacetato)rhodate(*III*)(1 −)



M 409.1 (ion)
Sol. H_2O.

H-compd., dihydrate:
$C_{10}H_{19}N_2O_{11}Rh$ M 446.1

Smith, B.B. *et al, Inorg. Chem.*, 1968, **7**, 2020 (*synth, pmr*)

$C_{10}H_{14}N_2O_9Ru^{\ominus}$ IC-006921

Aqua(ethylenediaminetetraacetato)ruthenate(*III*)(1 −)
Aqua[[N,N'-1,2-ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N',O,O',O^n,O^n']ruthenate(1 −), 9CI

[68122-22-5]

$[Ru[(OOCCH_2)_2NCH_2CH_2N(CH_2COO)_2](OH_2)]^{\ominus}$

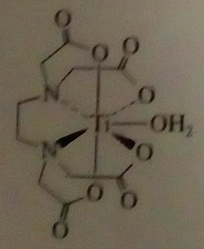
M 407.2 (ion)
One of many poorly characterised complexes of ruthenium(*III*) and [EDTA]$^{4\ominus}$. This is the form which predominates in aq. soln.; derived solids are usually hydrated. Struct. 6-coordinate, but undetermined. Prepd. by treating aq. $RuCl_3.xH_2O$ with $Na_2[H_2EDTA]$. Sol. H_2O.

Mukaida, M. *et al, Nippon Kagaku Zasshi (Jpn. J. Chem.)*, 1965, **86**, 598 (*synth*)
Ezerskaya, N.A. *et al, Russ. J. Inorg. Chem. (Engl. Transl.)*, 1966, **11**, 781, 991, 1168 (*chloro derivs*)
Shimizu, K. *et al, Bull. Chem. Soc. Jpn.*, 1974, **47**, 1651 (*synth, electrochem*)
Karmilov, A.Yu. *et al, Koord. Khim.*, 1977, **3**, 1079 (*reactions*)
Yoshino, Y. *et al, Bull. Chem. Soc. Jpn.*, 1979, **52**, 1060 (*reactions*)
Matsubara, T. *et al, Inorg. Chem.*, 1979, **18**, 1956 (*reaction*)
Saito, M. *et al, Bull. Chem. Soc. Jpn.*, 1980, **53**, 3531 (*synth*)
Ni, C.L. *et al, J. Electroanal. Chem. Interfacial Electrochem.*, 1986, **202**, 101 (*electrochem*)
Bajaj, H.C. *et al, Inorg. Chem.*, 1988, **27**, 4052 (*reactions*)
Ogino, H. *et al, Inorg. Chem.*, 1989, **28**, 3656 (*electrochem*)
Zhou, J. *et al, Inorg. Chem.*, 1990, **29**, 160 (*struct, electrochem*)

$C_{10}H_{14}N_2O_9Ti$ IC-006922

Aqua(ethylenediaminetetraacetato)titanium(*IV*)
Aqua[[N,N'-1,2-ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N',O,O',O^n,O^n']titanium(IV), 11CI

[96055-83-3]



M 354.1

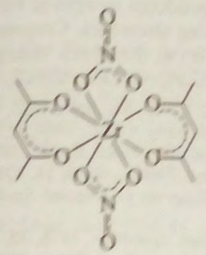
Pentagonal bipyramid. The equatorial plane occupied by H_2O, 2N and 2 carboxyl O's. Synth. from EDTA and an aq. soln. of $TiCl_4$ in HCl at pH1. Colourless solid. Sol. H_2O.

Fackler, J.P. *et al, Inorg. Chem.*, 1985, **24**, 1857 (*synth, cryst struct*)

$C_{10}H_{14}N_2O_{10}Zr$ IC-006923

Bis(nitrato-*O,O'*)bis(2,4-pentanedionato-*O,O'*)zirconium(*IV*), 11CI
Dinitratobis(2,4-pentanedionato)zirconium(IV), 9CI. Bis(nitrato-O)bis(2,4-pentanedioato-O,O')zirconium(IV), 10CI. Bis(acetylacetonato)dinitratozirconium(IV)

[21496-02-6]



M 413.4
Dodecahedron at Zr. Synth. from $ZrO(NO_3)_2.2H_2O$ and 2,4-pentanedione in C_6H_6. Colourless solid. Sol. C_6H_6/hexane.

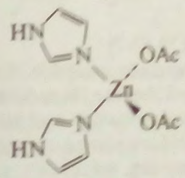
[56977-87-8]

Day, V.W. *et al, J. Am. Chem. Soc.*, 1975, **97**, 5136 (*synth, cryst struct*)
Fay, R.C. *et al, J. Am. Chem. Soc.*, 1979, **101**, 1115 (*synth, pmr*)

$C_{10}H_{14}N_4O_4Zn$ IC-006924

Bis(acetato-*O*)bis(1*H*-imidazole-*N*^{3})zinc
Bis(imidazole)zinc diacetate. Zinc(II) acetate bis(imidazole)

[74194-01-7]



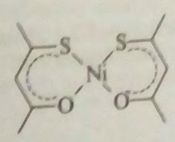
M 319.6
Comprises tetrahedral zinc in solid state. Cryst. (aq. EtOH). Insol. CCl_4.

Weze, G. *et al, Hoppe Seyler's Z. Physiol. Chem.*, 1956, **305**, 1 (*synth*)
Horricks, W.D. *et al, J. Inorg. Biochem.*, 1980, **12**, 131 (*synth, cryst struct*)
Horricks, W.D. *et al, Inorg. Chem.*, 1982, **21**, 3265.

$C_{10}H_{14}NiO_2S_2$ IC-006925

Bis(4-thioxo-2-pentanonato-*O,S*)nickel(*II*), 9CI
Bis(2-thio-2,4-pentanedionato)nickel(II), 8CI.
Bis(thioacetylacetonato)nickel(II)

[52612-96-1]



M 289.0
cis-Square planar. Deep brown cryst. Mp 168-169°.

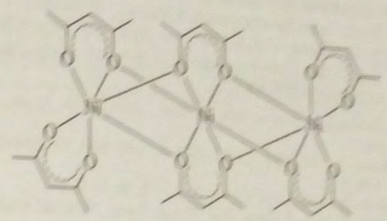
[14239-84-9]

Sinnan, O. *et al, J. Chem. Phys.*, 1971, **54**, 734 (*synth, pmr*)
Sinnan, O. *et al, J. Am. Chem. Soc.*, 1974, **96**, 2303 (*cryst struct, ir*)
Sinnan, O., *Inorg. Chem.*, 1980, **19**, 2989 (*spectra*)

$C_{10}H_{16}NiO_4$ IC-006926

Bis(2,4-pentanedionato-*O,O'*)nickel(*II*)
Bis(acetylacetonato)nickel(II). Nickel(II) acetylacetonate

[3264-82-2]



trimer

M 256.9
Trimeric in solid state with face-sharing octahedral Ni, not a monomer as commonly written. Best studied Ni diketonate. Pioneering ferromagnetic complex.

▶ SA2100000

Trimer: [12313-18-7]. *Hexakis(2,4-pentanedionato)trinickel(II)*
$C_{30}H_{42}Ni_3O_{12}$ M 770.7
Obt. by dehydration of Diaquabis(2,4-pentanedionato-*O,O'*)nickel(*II*), IC-007028 by vacuum subl. or azeotropic distillation with toluene. Commercially available. Forms many mononuclear and some dinuclear complexes. Catalyst for addition and polym. reactions. Green cryst. (C_6H_6). Sol. many org. solvs. Mp 229-230° dec., Mp 249° dec. $Subl._{0.2}$ 170°.

Tetramer: [53407-04-8]. *Octakis(2,4-pentanedionato)tetranickel*
$C_{40}H_{56}Ni_4O_{16}$ M 1027.6
Formed from solns. of trimer in CS_2.

Fieser and Fieser, Reagents for Organic Synthesis, **5**, 471; **6**, 417; **7**, 250; **8**, 42; **10**, 42 (*use*)
Inorg. Synth., 1957, **5**, 105, 1967, **10**, 5 (*synth*)
Johnson, A. *et al, J. Am. Chem. Soc.*, 1972, **94**, 1419 (*synth*)
Siegel, J.A. *et al, Inorg. Chim. Acta*, 1974, **9**, 19 (*tetramer*)
Schildcrout, S.M., *J. Phys. Chem.*, 1976, **80**, 2834 (*mol*)
Boyd, P.D.W. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 92 (*magnetism*)
Fragala, I. *et al, Inorg. Chim. Acta*, 1980, **40**, 15 (*pe*)
Hursthouse, M.B. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 307 (*cryst struct*)
Bhattacharjee, M.N. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2561 (*synth*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 143 (*reactions*)

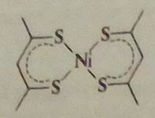
IC-006927

$C_{10}H_{14}NiS_4$

Bis(2,4-pentanedithionato-*S,S'*)nickel(*II*), 9CI, 8CI

Bis(dithioacetylacetonato)nickel(II). *Bis(dithio-2,4-pentanedionato)nickel*(II)

[10170-79-3]



M 321.1

Square planar monomeric struct. Se analogue also known. Synth. from Hexaaquanickel(*II*)(2+), IC-019897 + 2,4-pentanedione + H_2S. Dark red cryst. (Me_2CO). Mp >268° dec. Does not form 5- or 6-coord. complexes with potential ligands.

Barraclough, C.G. *et al*, *Aust. J. Chem.*, 1969, **22**, 891 (*synth, ir, pmr*)
Siiman, O. *et al*, *Inorg. Chem.*, 1969, **8**, 1846; 1980, **19**, 2889 (*ir, raman*)
Siiman, O. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 2652 (*uv*)
Beckett, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 622 (*cryst struct*)
Daktemieks, D.R. *et al*, *Org. Mass Spectrom.*, 1980, **15**, 556 (*ms*)

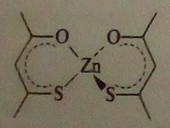
IC-006928

$C_{10}H_{14}O_2S_2Zn$

Bis(4-thioxo-2-pentanonato-*O,S*)zinc, 9CI

Bis(2-thio-2,4-pentanedionato)zinc

[15977-13-6]



M 295.7

Pale yellow needles (Me_2CO). Insol. H_2O. Mp 182-183°.

Yokoyama, A. *et al*, *Chem. Pharm. Bull.*, 1970, **18**, 356 (*synth*)
Belcher, R. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 1851 (*synth, ms*)
Bennett, A.M.A. *et al*, *Polyhedron*, 1989, **8**, 2305 (*ir, pmr, cmr*)

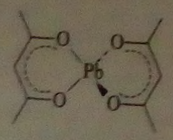
IC-006929

$C_{10}H_{14}O_4Pb$

Bis(2,4-pentanedionato-*O,O'*)lead, 9CI

Lead(II) *2,4-pentanedionate*. *Bis(acetylacetonato)lead*

[15282-88-9]



M 405.4

Synth. by heating PbO and 2,4-pentanedione in refluxing toluene. Pale yellow cryst. Mp 159° dec.

Schweitzer, G.K. *et al*, *Anal. Chim. Acta*, 1968, **43**, 332 (*synth*)
Gopinathan, C. *et al*, *Indian J. Chem.*, 1973, **11**, 1069 (*synth*)

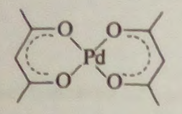
IC-006930

$C_{10}H_{14}O_4Pd$

Bis(2,4-pentanedionato-*O,O'*)palladium(*II*), 9CI

Bis(acetylacetonato)palladium. *Palladium*(II) *acetylacetonate*

[14024-61-4]



M 304.6

Square planar struct. Catalyses dimerisation of isoprene, carbonylation telomerisation and oligomerisation of dienes, vinylation of benzene derivs., dehydrogenation of chromanones and flavones, and carbonylation of epoxyalkenes; produces wet-proof Pd metal deposit on carbon-containing electrodes. Commercially available. Orange-yellow cryst. (benzene), orange-red cryst. (CH_2Cl_2). Sol. C_6H_6, CH_2Cl_2, $CHCl_3$. Mp 132-205° dec.

Sasaki, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 76 (*ms*)
McCarthy, P.J. *et al*, *Inorg. Chem.*, 1967, **6**, 781 (*synth, pmr*)
Knyazeva, A.N. *et al*, *Zh. Strukt. Khim.*, 1970, **11**, 938; *J. Struct. Chem. USSR (Engl. Transl.)*, 1970, **11**, 875 (*struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 45 (*use*)
Bulkin, B.J. *et al*, *Appl. Spectrosc.*, 1978, **32**, 151 (*ir, raman*)
Wilkie, C.A. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 195 (*cmr*)
Okeya, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 1085 (*synth, ir, pmr, cmr*)
Vlckova, B. *et al*, *Collect. Czech. Chem. Commun.*, 1985, **50**, 306 (*ir, raman*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **2**, 379, 390; **5**, 1114 (*reactions*)

IC-006931

$C_{10}H_{14}O_4Pt$

Bis(2,4-pentanedionato-*O,O'*)platinum(*II*), 8CI

Platinum(II) *acetylacetonate*. *Bis(acetylacetonato)platinum*

As Bis(1,1,1,5,5,5-hexafluoropentane-2,4-dionato)platinum, IC-006685 with

$X = CH_3$

M 393.2

Monomeric-form [15170-57-7]

Catalyst. Commercially available. Catalyses selective autooxidn. of cyclohexene, butadiene dimerisation, silicone rubber vulcanisation and alkene oxidn. Co-catalyst for hydroformylation reaction. Yellow cryst. (C_6H_6). Sol. many org. solvs.

Polymeric-form [32010-70-1]

Cream solid. Insol.

Lewis, J. *et al*, *J. Chem. Soc.*, 1965, 6740 (*ir, pmr*)
Sasaki, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 76 (*ms*)
Behnke, G.T. *et al*, *Inorg. Chem.*, 1967, **6**, 433 (*synth, ir*)
Gibson, D. *et al*, *J. Chem. Soc. A*, 1967, 72 (*polymer*)
Wilkie, C.A. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 195 (*cmr*)
Onuma, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 2679 (*struct*)
Inorg. Synth., 1980, **20**, 66 (*synth*)
U.S. Pat., 4 542 119, (1985); *CA*, **104**, 7496r (*use*)

IC-006932

$C_{10}H_{14}O_4Sn$

Bis(2,4-pentanedionato-*O,O'*)tin, 9CI

Bis(acetylacetonato)tin(II). *Tin*(II) *acetylacetonate*

[16009-86-2]

As Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O,O'*)tin, IC-006686 with

$R = CH_3$

M 316.9

Synth. by reaction of Sn(*II*) compds. with the β-diketone. Yellow viscous liq. d_4^{20} 1.49. Mp 18°. $Bp_{0.1}$ 105°. n_D^{20} 1.5775.

Ewings, P.F.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 821 (*synth, mössbauer, nmr, ms*)
Bos, K.D. *et al*, *J. Organomet. Chem.*, 1975, **99**, 397 (*synth*)
Wakeshima, I. *et al*, *Chem. Lett.*, 1981, 93 (*synth*)

IC-006933

$C_{10}H_{14}O_4Ti$

Bis(2,4-pentanedionato-*O,O'*)titanium(*II*), 11CI

Bis(acetylacetonato-O,O')*titanium*(II). *Titanium*(II) *acetylacetonate*

[20492-39-1]

$$[(H_3CCOCHCOCH_3)_2Ti]_n$$

M 246.0

Polymeric, perhaps like $Ni(acac)_2$. Synth. by reaction of Dichlorobis(2,4-pentanedionato-*O,O'*)titanium(*IV*), IC-006901 with Na in THF. Has limited use as a catalyst. Red-brown solid. Sol. THF, toluene, $CHCl_3$, Py; insol. H_2O, CCl_4, C_6H_6. Mp >300°. $Subl._{0.001}$ 200°. Paramagnetic: $\mu_{eff} = 0.41\mu_B$ (296K); $\mu_{eff} = 0.25\mu_B$ (90K).

Salzmann, J.-J., *Helv. Chim. Acta*, 1968, **51**, 601 (*synth, ir, uv-vis, magnetism*)
Japan. Pat., 78 73 225, (1978); *CA*, **89**, 147858g (*use*)
Fr. Pat., 2 493 835, (1982); *CA*, **98**, 4302w (*synth, use*)
Hurlocker, L.M., *Diss. Abstr. Int., B*, 1985, **46**, 541; *CA*, **103**, 89157x (*synth, use*)

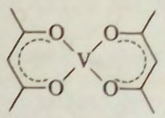
IC-006934

$C_{10}H_{14}O_4V$

Bis(2,4-pentanedionato-*O,O'*)vanadium(*II*), 11CI

Bis(acetylacetonato)vanadium(II). *Vanadium*(II) *acetylacetonate*

[14024-62-5]



M 249.1

Synth. from V(*II*) and 2,4-pentanedione in aq. soln. Polym. catalyst. Blue solid.

Schaefer, W.P., *Inorg. Chem.*, 1965, **4**, 642 (*synth*)
Barret, R. *et al*, *Bull. Soc. Chim. Belg.*, 1985, **94**, 157 (*use*)
Japan. Pat., 60 197 708, (1985); *CA*, **104**, 131212j (*use*)

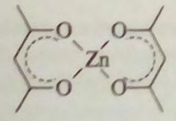
IC-006935

$C_{10}H_{14}O_4Zn$

Bis(2,4-pentanedionato-*O,O'*)zinc

Bis(acetylacetonato)zinc. *Zinc acetylacetonate*

[14024-63-6]



M 263.6

Monomeric in soln. Monomer is the metastable form. Polymerisation catalyst. Pvc stabiliser; cross-linking catalyst; trans-esterification catalyst. Cryst. (hexane). Sol. dry org. solvs. Mp 127°, Mp 152°. $Subl._{0.5}$ 60°. Forms a hydrate, Aquabis(2,4-pentanedionato-*O,O'*)zinc, IC-006994, which is dehydrated *in vacuo* over P_2O_5.

▷ ZH0920000

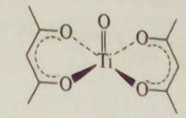
IC-006936

$C_{10}H_{14}O_5Ti$

Oxobis(2,4-pentanedionato-*O,O'*)titanium(*IV*), 11CI

Bis(acetylacetonato)oxotitanium(IV). *Titanyl acetoacetate*

[14024-64-7]



M 262.0

May be dimeric or polymeric. Synth. by atmospheric oxidation of $Ti(acac)_3$ or by electrochemical oxidation of Ti anodes in the presence of acac and O_2. Widely used as an epoxidation catalyst. Sol. C_6H_6. Insol. pet. ether.

▷ XR2330000.

Dimer: see *Di-μ-oxotetrakis(2,4-pentanedionato*-O,O')*dititanium*(IV), *IC-010587*

Homopolymer: [51866-75-2].

Synth. either from $(RO)_2Ti(acac)_2$ in weakly acidic H_2O or from a soln. of a Ti salt + H acac in H_2O at pH 2-7. Can be used as a crosslinking agent.

Cox, M. *et al*, *J. Chem. Soc.*, 1965, 2840 (*synth, ir*)
Japan. Pat., 74 07 226, (1974); *CA*, **81**, 26524w (*synth, homopolymer*)
Japan. Pat., 74 07 227, (1974); *CA*, **81**, 26523v (*synth, homopolymer, use*)
Grobe, J. *et al*, *Z. Naturforsch., B*, 1984, **39**, 808 (*electrochem synth*)
Bortolini, O. *et al*, *J. Mol. Catal.*, 1985, **33**, 241 (*use*)
U.S. Pat., 4 560 716, (1985); *CA*, **105**, 61753f (*use*)

Trimer: [15663-12-4]. *Tetrakis[μ-(2,4-pentanedionato-O:O,O')]bis(2,4-pentanedionato-O,O')trizinc*
$C_{30}H_{42}O_{12}Zn_3$ M 790.8
Formed on subl. of monomer. Cryst.

Lawson, K.R., *Spectrochim. Acta*, 1961, **17**, 248 (*ir*)
Graddon, D.P. *et al*, *Aust. J. Chem.*, 1963, **16**, 980 (*synth*)
Sasaki, S.-I. *et al*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 76 (*ms*)
Inorg. Synth., 1967, **10**, 74 (*synth*)
Bennett, M.J. *et al*, *Acta Crystallogr., Sect. B*, 1968, **24**, 904 (*cryst struct, trimer*)
Hammel, J.C. *et al*, *J. Chem. Soc. A*, 1969, 1401 (*pmr*)
Wilkie, C.A. *et al*, *J. Inorg. Nucl. Chem.*, 1978, **40**, 195 (*cmr*)
Shibata, S. *et al*, *J. Mol. Struct.*, 1981, **77**, 265 (*ed*)
Takegoshi, K. *et al*, *Inorg. Chem.*, 1987, **26**, 2552 (*solid-state cmr*)

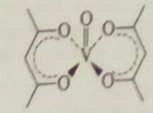
IC-006937

$C_{10}H_{14}O_5V$

Oxobis(2,4-pentanedionato-*O,O'*)vanadium(*IV*), 11CI

Bis(acetylacetonato)oxovanadium(IV). *Vanadyl acetylacetonate*

[3153-26-2]



M 265.1

Square pyramidal. Synth. by refluxing V_2O_5 and 2,4-pentanedione. Commercially available. Catalyst component for a very wide range of reactions. Has also been widely used for uv-vis and esr spectral studies. Blue cryst. Sol. EtOH, C_6H_6, $CHCl_3$. Readily forms adduct esp. with N-donors.

Py complex: [24263-31-8]. *(Acetylacetonato)oxo(pyridine) vanadium*(IV)
Synth. by dissolving $VO(acac)_2$ in Py. Green cryst. Sol. org. solvs.; insol. H_2O. Ir ν_{VO} 995 cm^{-1}.

Aniline complex: [68021-28-1]. *Bis(acetylacetonato)(aniline) oxovanadium(IV)*. (*Benzenamine*)*oxobis(2,4-pentanedionato-O,O′)vanadium*(IV), *11CI*

No phys. props. reported.

Ethanolamine complex: [68021-28-0]. (*2-Aminoethanol-N*)*oxobis(2,4-pentanedionato-O,O′)vanadium*(IV), *11CI*

[14284-84-5, 88271-97-9]

Inorg. Synth., 1957, **5**, 115 (*synth*)

Dodge, R.P. *et al*, *J. Chem. Phys.*, 1961, **35**, 55 (*cryst struct*)

Hon, P. *et al*, *J. Chem. Phys.*, 1965, **43**, 3111 (*cryst struct*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 458; 1972, **3**, 331; 1984, **11**, 47; 1986, **12**, 63; 1988, **13**, 54 (*uses*)

Adachi, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 401 (*synth, uv-vis, Py complex*)

Kivisto, R. *et al*, *J. Phys. Chem.*, 1982, **86**, 2743 (*endor*)

Urbanovych, A. *et al*, *Monatsh. Chem.*, 1983, **114**, 1311 (*uv-vis, esr*)

Macazaga, M.J. *et al*, *Transition Met. Chem.*, 1983, **8**, 215 (*Py complex, uv-vis, thermn constn*)

Shao, M. *et al*, *Kexue Tongbao (Foreign Lang. Ed.)*, 1984, **29**, 759; *CA*, **101**, 161589n (*cryst struct, Py complex*)

Martinez, J. *et al*, *Thermochim. Acta*, 1985, **87**, 281 (*Py complex, synth, ir, thermal props*)

Astashkin, A.V., *Zh. Strukt. Khim.*, 1985, **26**, 53; *CA*, **103**, 225995y (*synth, esr, detns*)

$C_{10}H_{14}O_5U$ IC-006938

Dioxobis(2,4-pentanedionato-*O,O′*)uranium(*VI*), 11CI

Uranyl acetylacetonate

[18039-69-5]

As Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O,O′*) dioxouranium(*VI*), IC-006688 with

$R^1 = R^2 = CH_3$

M 468.2

Used in synth. of photomasks. Catalyst in synth. of polybutadiene, polyisoprene, etc. Added to PVC to reduce smoke emission during combustion. V. moisture-sensitive orange to yellow-orange cryst. Sol. toluene, C_6H_6, Me_2CO, CCl_4, EtOH, MeOH. Mp 225° (230-235° dec.). Ms shows monomer in vapour. Ir $\nu_{U=O}$ 925 cm^{-1}. Forms adducts with range of amine and other donors.

Monohydrate: [18701-96-7]. *Aquadioxobis(pentanedionato-O,O′)uranium*(VI). *Uranyl acetate hydrate*

Yellow to orange-yellow cryst. Sol. Et_2O, dichloroethane, toluene. Ir $\nu_{U=O}$ 925-910 cm^{-1}. Four cryst. forms known. Pentagonal bipyramidal struct. Loses H_2O over P_2O_5 at 110°.

2,4-Pentanedione complex:

$C_{15}H_{22}O_6U$ M 568.3

Light orange cryst. Sol. acetylacetone. 7-Coord. pentagonal bipyramid.

2-Amino-4-pentanone complex (*1:1*): [69692-13-3].

Yellow cryst. 7-Coord. pentagonal bipyramid.

2-(N-Methylamino)-4-pentanone complex: [33196-70-2].

Yellow cryst. 7-Coord. pentagonal bipyramid.

Py complex: [33701-13-2]. *Dioxobis(2,4-pentadionato-O,O′)(pyridine)uranium*

$C_{15}H_{19}NO_6U$ M 547.3

Orange-yellow cryst. (MeOH). Sol. MeOH, EtOH. Has bent uranyl group (173.5°) due to steric effects.

Biltz, W. *et al*, *Z. Anorg. Allg. Chem.*, 1904, **40**, 221 (*synth, hydrate*)

Hager, K., *Z. Anorg. Allg. Chem.*, 1927, **162**, 82 (*synth, py complex*)

Abrahamson, E.W., *J. Am. Chem. Soc.*, 1950, **72**, 1424 (*synth, hydrate*)

Schlesinger, H.I. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 2446 (*synth, up*)

Sacconi, L. *et al*, *J. Chem. Soc.*, 1958, 4257.

Comyns, A.E. *et al*, *J. Chem. Soc.*, 1958, 4633 (*synth, ir, hydrate, uv*)

Sacconi, L. *et al*, *J. Inorg. Nucl. Chem.*, 1958, **8**, 93 (*ir, hydrate, py complex*)

Calino, A., *Gazz. Chim. Ital.*, 1959, **89**, 939 (*synth*)

Belford, R.L. *et al*, *J. Inorg. Nucl. Chem.*, 1960, **14**, 169 (*synth, uv-vis*)

Fraxson, E. *et al*, *Nature (London)*, 1964, **202**, 1325 (*cryst struct, hydrate*)

Jones, M.M. *et al*, *J. Inorg. Nucl. Chem.*, 1965, **25**, 369 (*props*)

Fraxson, E. *et al*, *Coord. Chem. Rev.*, 1966, **1**, 145 (*cryst struct, hydrate*)

Berg, E.W. *et al*, *Anal. Chim. Acta*, 1968, **40**, 101 (*synth*)

U.S. Pat., 3676411, (1970); *CA*, **77**, 103037 (*use*)

Haigh, J.M. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **37**, 1787 (*synth, pmr, ir*)

Issa, J.M. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 505 (*synth, use*)

Clemente, D.A. *et al*, *J. Cryst. Mol. Struct.*, 1973, **3**, 221 (*cryst struct*)

Haigh, J.M. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 1398 (*complex, cryst struct*)

Rodgers, A.L. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 3110 (*complex, cryst struct*)

Fragala, I. *et al*, *Inorg. Chem.*, 1978, **17**, 3175 (*mx, pe*)

Lenner, M. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 2396 (*complex, cryst struct*)

Japan. Pat., 57 104 933, (1982); *CA*, **98**, 135309 (*use*)

Alcock, N.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 679 (*synth, cryst struct, py complex*)

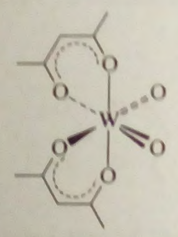
Bhattacharjee, M.N. *et al*, *Int. J. Mass Spectrom. Ion Phys.*, 1986, **71**, 109 (*ms*)

$C_{10}H_{14}O_6W$ IC-006939

Dioxobis(2,4-pentanedionato-*O,O′*)tungsten(*VI*)

Bis(acetylacetonato)dioxotungsten(IV)

[21292-49-9]



M 414.0

WO_2 unit shown to be bent by ir. Synth. from $WO_2Cl_2(OPPh_3)_2$ and 2,4-pentanedione. Pale yellow solid.

Nikolovski, A., *Croat. Chim. Acta*, 1968, **40**, 143.

Soptrajanov, B. *et al*, *Spectrochim. Acta, Part A*, 1968, **24**, 1617 (*ir*)

Rice, C.A. *et al*, *Inorg. Chem.*, 1981, **20**, 1996 (*synth, ir*)

McDonell, A.C. *et al*, *Aust. J. Chem.*, 1985, **38**, 1017.

$C_{10}H_{14}O_{10}Pb_2S_4$ IC-006940

(Ethanediylidenetetrathiotetraacetato)lead(*II*) dihydrate

2,2′,2″,2‴-[1,2-Ethanediylidenetetrakis(thio)]tetrakis[acetic acid] lead(2+) salt (1:2) dihydrate, *9CI*

[77182-59-3]

$[(O_2CCH_2S)_2CHCH(SCH_2CO_2)_2]^{4\ominus}.2Pb^{2\oplus}.2H_2O$

M 836.8

Cryst.

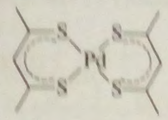
Houttemane, C. *et al*, *Acta Crystallogr., Sect. B*, 1981, **37**, 686 (*cryst struct*)

$C_{10}H_{14}PdS_4$ IC-006941

Bis(2,4-pentanedithionato-*S,S′*)palladium(*II*)

Bis(dithioacetylacetonato)palladium(II)

[10170-80-6]



M 368.9

Bright red cryst. (Me_2CO). Sol. org. solvs.; insol. H_2O. Mp 240°.

Martin, R.L. *et al*, *Nature (London)*, 1966, **210**, 522 (*synth, ir, uv*)

Simann, O. *et al*, *Inorg. Chem.*, 1969, **8**, 1846 (*synth, ir*)

$C_{10}H_{15}AlBrN_5^{2\oplus}$ IC-006942

Pentakis(acetonitrile)bromoaluminium(2+)

[62389-67-7]

$[AlBr(NCCH_3)_5]^{2\oplus}$

M 312.1 (ion)

Detected by nmr in solns. of $AlBr_3$ in MeCN. Several similar spp. descr.

Akitt, J.W. *et al*, *J. Magn. Reson.*, 1977, **25**, 391 (*Al-27 nmr*)

Dalibart, M. *et al*, *Inorg. Chem.*, 1981, **20**, 3975 (*Al-27 nmr*)

Wehrli, F.W. *et al*, *J. Magn. Reson.*, 1981, **44**, 197 (*Al-27 nmr*)

$C_{10}H_{15}AlClN_5^{2\oplus}$ IC-006943

Pentakis(acetonitrile)chloroaluminium(2+)

[60475-07-2]

$[AlCl(NCCH_3)_5]^{2\oplus}$

M 267.6 (ion)

Detected in solns. of $AlCl_3$ in MeCN. Several related ions descr.

Bis-tetrachloroaluminate(*1−*), *compd. with MeCN* (*1:1*): [60475-09-4]. *Aluminium trichloride-bis(methylcyanide)*

$C_{12}H_{18}Al_3Cl_9N_6$ M 646.3

Synth. from $AlCl_3$ and an excess of MeCN. Colourless moisture sensitive cryst. (MeCN). C.f. Aluminium(*III*) chloride ($AlCl_3$), IC-000132.

Howard, J.A.K. *et al*, *J. Chem. Soc., Chem. Commun.*, 1976, 477 (*cryst struct*)

Akitt, J.W. *et al*, *J. Magn. Reson.*, 1977, **25**, 391; 1979, **34**, 435 (*Al-27 nmr*)

Beattie, I.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 528 (*Al-27 nmr, Cl-35 nmr, raman, conductivity, cryst struct*)

Wehrli, F.W. *et al*, *J. Magn. Reson.*, 1981, **42**, 334; **44**, 197 (*Al-27 nmr*)

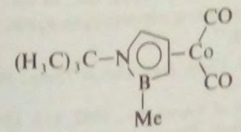
Dalibart, M. *et al*, *Inorg. Chem.*, 1982, **21**, 1040, 2241 (*Al-27 nmr, ir, raman*)

$C_{10}H_{15}BCoNO_2$ IC-006944

Dicarbonyl[(3,4,5-η)-1-(1,1-dimethylethyl)-2,3-dihydro-2-methyl-1*H*-1,2-azaborol-3-yl-*B*²,*N*¹]cobalt, 11CI

(1-tert-Butyl-2,5-dihydro-2-methyl-η⁵-1H-1,2-azaborolyl) dicarbonylcobalt

[100938-85-0]



M 250.9

Red oil. Sol. C_6H_6, pet. ether. $Bp_{0.001}$ 80-90°. Ir ν_{CO} 2020, 1955 cm^{-1} (pentane).

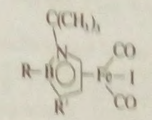
Schmid, G. *et al*, *Chem. Ber.*, 1986, **119**, 1766 (*synth, ir, pmr, cmr, B-11 nmr, ms, props*)

$C_{10}H_{15}BFeINO_2$ IC-006945

[(3,4,5-η)-1-*tert*-Butyl-2,3-dihydro-2-methyl-1*H*-1,2-azaborol-3-yl-*B*³,*N*²]iodoiron

Dicarbonyl[(3,4,5-η)-1-(1,1-dimethylethyl)-2,3-dihydro-2-methyl-1H-1,2-azaborol-3-yl-B²,N²]iodoiron, *10CI*

[75334-22-4]



R = Me, R′ = H

M 374.7

Red-brown cryst. (pet. ether). Mp 87-88°.

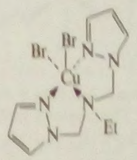
Schulze, J. *et al*, *J. Organomet. Chem.*, 1980, **193**, 83 (*synth, ms, ir, pmr, nmr*)

$C_{10}H_{15}Br_2CuN_5$ IC-006946

[*N,N*-Bis(pyrazol-1-ylmethyl)aminoethane-*N,N′,N″*] dibromocopper(*II*)

Dibromo[N-*ethyl*-N-(1H-*pyrazol-1-ylmethyl*)-1H-*pyrazole-1-methanamine*]*copper*(II), *11CI*

[103079-80-7]



M 428.6

Distorted square pyramidal geometry. Cu-apical Br 267 pm. Dark green cryst. (MeOH).

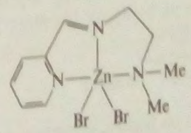
Veldhuis, J.B.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 537 (*synth, ir, esr, cryst struct, uv*)

$C_{10}H_{15}Br_2N_3Zn$ IC-006947

Dibromo[2-[[2-(dimethylamino)ethyl]amino]methyl] pyridine]zinc

Dibromo[1-(2-*pyridyl*)-2,5-*diaza*-5-*methylhexene*]*zinc*

[29987-32-4]



M 402.4

Coordination configuration is a distorted trigonal bipyramid. Prepd. from $Me_2NCH_2CH_2NH_2$ + 2-pyridinecarboxaldehyde + $ZnBr_2$ in boiling EtOH. White cryst. ($CHCl_3/Me_2CO$).

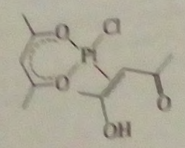
Zakrzewski, G. *et al*, *Inorg. Chim. Acta*, 1970, **4**, 251 (*synth, cryst struct*)

$C_{10}H_{15}ClO_4Pt$ IC-006948

Chloro(2,4-pentanedionato)(2,4-pentanedione)platinum(*II*)

Chloro(4-hydroxy-3-penten-2-one)(2,4-pentanedionato)platinum

[33269-54-4]



M 429.7

Unusual example of enol form of diketone acting as an alkene ligand. Synth. by acidification of Chlorobis(2,4-pentanedionato)platinate(*II*)(1−), IC-006891. Yellow solid. Sol. C_6H_6, $MeNO_2$. Br analogue also known.

[12129-03-2]

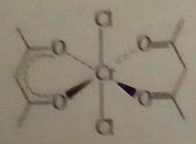
Gibson, D. *et al*, *J. Chem. Soc. A*, 1967, 72 (*synth, ir, pmr*)
Behnke, G.T. *et al*, *Inorg. Chem.*, 1968, **7**, 2030 (*ir*)

$C_{10}H_{15}Cl_2CrO_4$ IC-006949

Dichloro(2,4-pentanedionato-*O,O'*)(2,4-pentanedione-*O,O'*)chromium(*III*), 9Cl

(Acetylacetonato)(acetylacetone)dichlorochromium(III)

[37581-70-9]



M 322.1

trans-Octahedral struct. based on ir data. V. hygroscopic pale green solid. Thermodynamically rather unstable. Sol. 2,4-pentanedione. $\mu_{eff} = 3.96\mu_B$ (293K).

Nakamura, Y. *et al*, *Inorg. Chem.*, 1972, **11**, 1573 (*synth, magnetism, rpa, ir, uv-vis*)

$C_{10}H_{15}CoN_5^{\oplus}$ IC-006950

Pentakis(isocyanomethane)cobalt(1+), 10Cl

Pentakis(methylisonitrile)cobalt(1+), Pentakis(methyl isocyanide)cobalt(1+)

[14024-66-9]

$[(MeNC)_5Co]^{\oplus}$

M 284.1 (ion)

Perchlorate: Yellow cryst. (MeOH). Mp 152°.
▷ Dec. violently on heating or percussion or in contact with oxidising agents.

Tetracarbonylcobaltate:
$C_{14}H_{15}Co_2N_5O_4$ M 435.1
Yellow cryst.
▷ Dec. violently on heating, percussion or contact with oxidising agents.

Hexafluorophosphate: Yellow cryst.

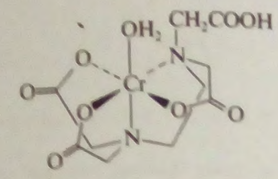
Hieber, W. *et al*, *Chem. Ber.*, 1954, **87**, 789 (*synth*)
Sacco, A. *et al*, *Gazz. Chim. Ital.*, 1959, **89**, 1800 (*synth*)
Cotton, F.A. *et al*, *Inorg. Chem.*, 1965, **4**, 318 (*cryst struct*)
Boorman, P.M. *et al*, *Can. J. Chem.*, 1970, **48**, 838 (*ir, raman*)
Baltch, A.L., *J. Am. Chem. Soc.*, 1976, **98**, 285
Kawakami, K. *et al*, *J. Inorg. Nucl. Chem.*, 1979, **41**, 1501 (*reactions*)

$C_{10}H_{15}CrN_2O_9$ IC-006951

Aqua(ethylenediaminetriacetato-acetic acid)chromium(*III*)

Aqua[[1,2-ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N',O,O',O^N]chromate(1−) hydrogen, 10Cl

[76582-41-7]



M 359.2

Distorted octahedral coordination about Cr. Extensive H-bonding observed between molecules. Synth. from Na_2(edta) and $Cr(NO_3)_3$. Violet cryst. (aq. dioxan).

[15955-81-4]

Hamm, R.E., *J. Am. Chem. Soc.*, 1953, **75**, 5670 (*synth, uv-vis*)
Gerdom, L.E. *et al*, *Inorg. Chem.*, 1981, **20**, 1606 (*cryst struct*)

$C_{10}H_{15}CrN_6O^{\oplus}$ IC-006952

Pentakis(isocyanomethane)nitrosylchromium(1+), 11Cl, 9Cl

Pentakis(methyl isocyanide)nitrosylchromium(1+)

$[Cr(NO)(CNMe)_5]^{\oplus}$

M 287.2 (ion)

Octahedral cation. Starting material. Many tertiary phosphine-substituted derivs. known. Can be oxidised to (2+) cation.

Tetrafluoroborate: [86968-76-5].
Synth. from MeNC in excess and $[Cr(NO)(NCMe)_5](BF_4)_2$.

Hexafluorophosphate: [51406-89-4].
Synth. by reduction of $[Cr(NO)(CNMe)_5](PF_6)_2$ or MeNC on $[Cr(NO)_2(NCMe)_4](PF_6)_2$. Violet cryst. $(CHCl_3)$. Re-oxidised by $AgNO_3/KPF_6$. Diamagnetic. Ir ν_{NO} 1675 cm^{-1}.

Lloyd, M.K. *et al*, *J. Organomet. Chem.*, 1973, **61**, 261 (*synth, ir*)
Herberhold, M. *et al*, *Chem. Ber.*, 1982, **115**, 1399.
Wigley, D.E. *et al*, *Organometallics*, 1982, **1**, 1322 (*synth, electrochem*)
Pierce, J.L. *et al*, *Organometallics*, 1982, **1**, 1328 (*synth, ms*)
Wigley, D.E. *et al*, *Inorg. Chem.*, 1983, **22**, 3138 (*synth*)
Robinson, W.R. *et al*, *Inorg. Chem.*, 1985, **24**, 918.

$C_{10}H_{15}CrN_6O^{2\oplus}$ IC-006953

Pentakis(acetonitrile)nitrosylchromium(2+), 11Cl, 10Cl

$[Cr(NO)(NCMe)_5]^{2\oplus}$

M 287.2 (ion)

Octahedral cation. Acetonitrile may be displaced by P- and S-donor ligands. Starting material.

Bis-tetrafluoroborate: [75845-06-6].
Synth. from $Cr(CO)_6$ in MeCN + $NOBF_4$ in excess.

Bis-hexafluorophosphate: [75661-39-1].
Synth. from $Cr(CO)_6$ in MeCN + $NOPF_6$ in excess. Yellow solid ($MeCN/Et_2O$); dec. in air. Sol. Me_2CO, MeCN giving yellow air-sensitive solns. Ir ν_{NO} 1797, ν_{CN} 2328, 2307 cm^{-1}.

Clamp, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 2162 (*synth, ir, esr*)
Herberhold, M. *et al*, *Chem. Ber.*, 1982, **115**, 1399 (*synth, ir*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 826 (*rev*)

$C_{10}H_{15}CrN_6S^{2\oplus}$ IC-006954

Pentakis(acetonitrile)thionitrosylchromium(2+), 10Cl

$[Cr(NS)(NCCH_3)_5]^{2\oplus}$

M 303.3 (ion)

Approx. octahedral at Cr.

Bis-hexafluorophosphate: [75661-37-9].
Blue cryst. ($MeCN/Et_2O$).

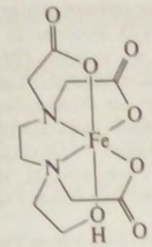
Herberhold, M. *et al*, *Z. Naturforsch., B*, 1980, **35**, 1277 (*synth, ir*)

$C_{10}H_{15}FeN_2O_7$ IC-006955

[*N*-[2-[Bis(carboxymethyl)amino]ethyl]-*N*-(2-hydroxyethyl)glycinato(3−)]iron(*III*), 11Cl

[N-(Carboxymethyl)-N'-2-(hydroxymethyl)-N,N'-ethylenediglycinato(3−)]iron, 8Cl

[17084-02-5]



M 331.0

Usually obt. hydrated. Structure and presence of coordinated water uncertain. Synth. from $FeCl_3$ + H_3L + NaOH. Used for removal of H_2S from gas streams. Amber cryst. $\mu_{eff} = 5.85\mu_B$. Closely related to (Ethylenediaminetetraacetato)ferrate(*III*)(1−), IC-006856.

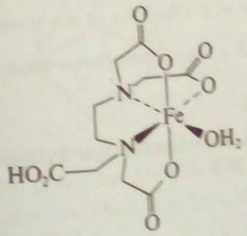
Gustafson, R.L. *et al*, *J. Phys. Chem.*, 1963, **67**, 576 (*reactions*)
Kornev, V.E. *et al*, *Zh. Fiz. Khim.*, 1967, **41**, 1378 (*formn, uv-vis*)
Schugar, H.J. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 1419 (*synth, mössbauer, ir, uv*)
Stein, G.E. *et al*, *J. Inorg. Nucl. Chem.*, 1975, **37**, 2421 (*synth, mössbauer*)

$C_{10}H_{15}FeN_2O_9$ IC-006956

Aqua[ethylenediamine-*N,N,N',N'*-tetraacetato(3−)]iron(*III*)

Aqua[[1,2-ethanediyldinitrilotetraacetato](3−)]iron(III)

[47175-70-2]



M 363.0

Octahedral Fe. Yellow cryst. + $1H_2O$ (H_2O). Sol. H_2O.

[103130-21-8]

Kennard, C.H.L., *Inorg. Chim. Acta*, 1967, **1**, 347 (*struct*)

$C_{10}H_{15}FeO_7P$ IC-006957

Tetracarbonyl(triethyl phosphite-*P*)iron, 9Cl

Tetracarbonyl(phosphorous acid)iron triethyl ester, 8Cl

[21494-36-0]

$(EtO)_3PFe(CO)_4$

M 334.0

Pale-yellow liq. $Bp_{0.1}$ 100°.

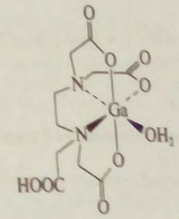
Cotton, J.D. *et al*, *Aust. J. Chem.*, 1969, **22**, 2673 (*synth, ir, pmr, ms, raman*)
Udovich, C.A. *et al*, *Inorg. Chem.*, 1969, **8**, 1066 (*stereochem*)
Greatrex, R. *et al*, *J. Organomet. Chem.*, 1976, **14**, 199 (*mössbauer*)

$C_{10}H_{15}GaN_2O_9$ IC-006958

Aqua(hydrogen ethylenediaminetetraacetato)gallate(*III*)

Aqua[(ethylenedinitrilo)tetraacetato(3−)-N,N',O,O']gallium(III)

[21199-67-7]



M 376.9

Approx. octahedral at Ga. Synth. from EDTA and aq. Ga(*III*). Colourless cryst. (H_2O).

Kennard, C.H.L., *Inorg. Chim. Acta*, 1967, **1**, 347 (*cryst struct*)
Clevette, D.J. *et al*, *Polyhedron*, 1990, **9**, 151 (*thermodyn props*)

$C_{10}H_{15}MnN_6O^{2\oplus}$ IC-006959

Pentakis(isocyanomethane)nitrosylmanganese(2+), 9Cl

Pentakis(methyl isocyanide)nitrosylmanganese(II)

$[Mn(CNMe)_5NO]^{2\oplus}$

M 290.2 (ion)

Bis-fluorosulfate: [42584-10-1].
Synth. from $K_3[Mn(NO)(CN)_5]$ and $MeOSO_2F$. No physical data available.

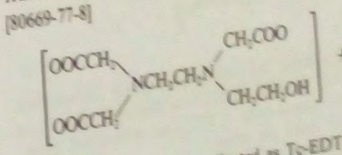
Eaborn, C. *et al*, *J. Organomet. Chem.*, 1973, **55**, C68 (*synth*)

$C_{10}H_{15}N_2O_7Tc$ IC-006960

[*N*-(2-Hydroxyethyl)ethylenediaminetriacetato]technetium(*III*)

HEDTA-Tc: [*N*-[2-[Bis(carboxymethyl)amino]ethyl]-*N*-(2-hydroxyethyl)glycinato(3−)]technetium, 9Cl. *Technetium - HEDTA*

[80669-77-8]



M 374.1

This system may be as complicated as Tc-EDTA system but has been very much less investigated. A cationic Tc-HEDTA complex has also been described. Sol. H_2O.

Eckelman, W. *et al*, *J. Nucl. Med.*, 1971, **12**, 596 (*synth*)
Yoshihara, K. *et al*, *Radiochim. Acta*, 1981, **28**, 131 (*synth, props*)

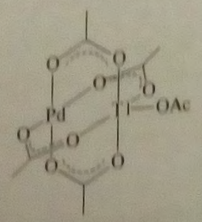
$C_{10}H_{15}O_{10}PdTl$ – $C_{10}H_{16}As_2Cl_4Pd$

$C_{10}H_{15}O_{10}PdTl$ IC-006961

Tetrakis(μ-acetato)(acetatothallium)palladium, 10Cl(*II*)

[*Acetatothallium*(III)]*tetra-μ-acetatopalladium*(II). *Palladium*(II) *thallium*(III) *acetate*

[74114-13-9]



M 606.0

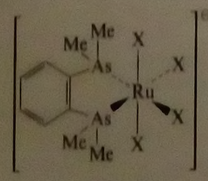
Probable struct. shown. Synth. from $[Pd_3(OAc)_6]$ + $Tl(OAc)_3$. Orange cryst. (hexane). Sol. hexane, $CHCl_3$. Several analogous compds. for other carboxylates known.

van der Ploeg, A.F.M.J. *et al*, *Inorg. Chim. Acta*, 1980, **38**, 253 (*synth, pmr, cmr*)

$C_{10}H_{16}As_2Br_4Ru^{\ominus}$ IC-006962

Tetrabromo[1,2-phenylenebis[dimethylarsine]-*As,As'*] ruthenate(*III*)(1−)

[*1,2-Bis*(*dimethylarsino*)*benzene*]*tetrabromoruthenate*(III)



X = Br

M 706.7 (ion)

cis-Octahedral form known only.

Dibromobis[*1,2-phenylenebis*[*dimethylarsine*]-As,As'] *ruthenium*(*1+*) *salt*:

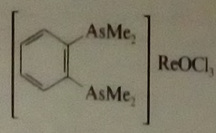
$C_{30}H_{48}As_6Br_6Ru_2$ M 1539.8

Prepd. by oxidising Ru(*II*) analogue with Br_2 in $CHCl_3$. Green salt. Mp 258° dec. μ_{eff} = 1.97μ_B (per Ru atom).

Nyholm, R.S. *et al*, *J. Chem. Soc.*, 1958, 567 (*synth, magnetism*)

$C_{10}H_{16}As_2Cl_3ORe$ IC-006963

Trichlorooxo[1,2-phenylenebis(dimethylarsine)-*As,As'*] rhenium(*V*)



M 594.6

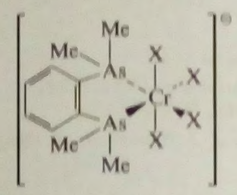
Approx. octahedral but detailed stereochem not reported. Synth. from $Re(CO)_3$(diars)Cl by treatment with Cl_2 in hot EtOH. Green cryst. ($CHCl_3$/pet. ether). Sol. most org. solvs.; insol. pet. ether.

Kirkham, W.J. *et al*, *J. Chem. Soc.*, 1965, 550 (*synth, ir, conductivity*)

Fergusson, J.E., *Coord. Chem. Rev.*, 1966, **1**, 459 (*rev, bibl*)

$C_{10}H_{16}As_2Cl_4Cr^{\ominus}$ IC-006964

Tetrachloro[1,2-phenylenebis[dimethylarsine]-*As,As'*] chromate(*III*)(1−), 11Cl



X = Cl

M 479.8 (ion)

Octahedral. Several analogues also known.

Tetrapropylammonium salt: [82456-77-7].

Synth. from $Cr(THF)_3Cl_3$, $[NPr_4]Cl$ and *o*-$C_6H_4(AsMe_2)_2$ in CH_2Cl_2. Blue moisture-sensitive solid. Sl. sol. CH_2Cl_2, toluene; dec. by H_2O, alcohols. Ir ν_{Cr-Cl} 358sh, 333m, 325s, 312sh cm^{-1}. μ_{eff} = 3.9μ_B (293K).

Dichlorobis[*1,2-phenylenebis*[*diphenylarsine*]-As,As'] *chromium*(*1+*) *salt*: see *Dichlorobis*[*1,2-phenylenebis*[*dimethylarsine*]-As,As']*chromium*(III) (*1+*),*11Cl*, *IC-010626*

Hale, A.L. *et al*, *Inorg. Chem.*, 1982, **21**, 3570 (*synth, ir, uv*)

Hale, A.L. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2569 (*synth, ir, uv*)

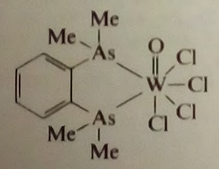
Gray, L.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2573 (*synth, ir, uv*)

Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 852 (*rev*)

$C_{10}H_{16}As_2Cl_4OW$ IC-006965

Tetrachlorooxo[1,2-phenylenebis(dimethylarsine)] tungsten(*VI*)

[27459-53-6]



M 627.7

7-Coordinate pentagonal bipyramid. Synth. from the diarsine and $WOCl_4$ in CCl_4. Green cryst., stable towards air, H_2O and org. solvs. Diamagnetic, Ir $\nu_{W=O}$ 964 cm^{-1}. Non-electrolyte.

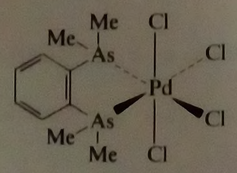
Drew, M.G.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 292 (*cryst struct*)

Blight, D.G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 313 (*synth*)

$C_{10}H_{16}As_2Cl_4Pd$ IC-006966

Tetrachloro[1,2-phenylenebis[dimethylarsine]-*As,As'*] palladium(*IV*), 9Cl

[85744-77-0]



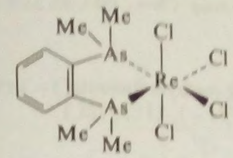
M 534.3

Orange solid.

Gray, L.R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 133 (*synth, ir*)

$C_{10}H_{16}As_2Cl_4Re$ IC-006967

Tetrachloro[1,2-phenylenebis(dimethylarsine)-*As,As'*] rhenium(*IV*)



M 614.0

Synth. from $Re(CO)_3$(diars)Cl and Cl_2 in CCl_4. Mustard-yellow cryst. ($CHCl_3$/pet. ether). Sol. C_6H_6, $CHCl_3$, $PhNO_2$.

Kirkham, W.J. *et al*, *J. Chem. Soc.*, 1965, 550 (*synth, props*)

$C_{10}H_{16}As_2Cl_4Ru^{\ominus}$ IC-006968

Tetrachloro[1,2-phenylenebis[dimethylarsine]-*As,As'*] ruthenate(1−)

[*1,2-Bis*(*dimethylarsino*)*benzene*]*tetrachlororuthenate*(III)

[94485-18-4]

As Tetrabromo[1,2-phenylenebis[dimethylarsine]-*As,As'*] ruthenate(*III*)(1−), IC-006962 with

X = Cl

M 528.9 (ion)

Dichlorobis[*1,2-phenylenebis*[*dimethylarsine*]-As,As'] *ruthenium*(*1+*) *salt*:

$C_{30}H_{48}As_6Cl_6Ru_2$ M 1273.0

Prepd. by oxidising ruthenium(*II*) analogue with Cl_2 in $CHCl_3$. Blue-green salt. Mp 233° dec. μ_{eff} = 1.86μ_B (per Ru atom).

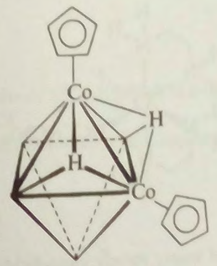
Nyholm, R.S. *et al*, *J. Chem. Soc.*, 1958, 567 (*synth, magnetism*)

$C_{10}H_{16}B_4Co_2$ IC-006969

Bis(η⁵-2,4-cyclopentadien-1-yl)[μ-[(*H'*,1,2,3-η:*H*⁴,2,3,4-η)-hexahydrotetraborato-(4−)]]dicobalt, 11Cl

1,2-Bis(*cyclopentadienylcobalt*)*hexaborane*(*6*)

[50924-50-0]



M 297.3

closo-. Dark red cryst. Sol. Me_2CO, $CHCl_3$.

Miller, V.R. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 5078; 1977, **99**, 5646 (*B-11 nmr, pmr*)

Weiss, R. *et al*, *Inorg. Chem.*, 1978, **17**, 1522 (*synth*)

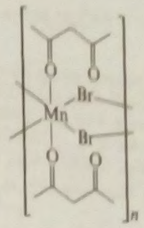
Pipal, J.R. *et al*, *Inorg. Chem.*, 1979, **18**, 252 (*cryst struct*)

$C_{10}H_{16}Br_2MnO_4$ IC-006970

Dibromobis(2,4-pentanedione-*O*)manganese(*II*)

Bis(*acetylacetone*)*dibromomanganese*(II)

[33960-62-2]



M 414.9

Polymeric chain struct. with octahedral Mn and bridging Br. Synth. eg. from anhydrous $MnBr_2$ and 2,4-pentanedione. Hygroscopic pale pink-colourless cryst.

[55025-70-2]

Koda, S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1971, 280 (*synth, cryst struct, magnetism*)

Nakamura, Y. *et al*, *Inorg. Chem.*, 1972, **11**, 1573 (*magnetism, ir*)

Isobe, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 250 (*synth*)

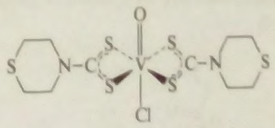
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 64 (*rev, bibl*)

$C_{10}H_{16}ClN_2OS_6V$ IC-006971

Chlorobis(4-thiomorpholinecarbodithioato-S^4,S^4) oxovanadium(*V*), 11Cl

Chlorobis(*1,4-thiazanecarbodithioato*-S^4,S^4)*oxovanadium*(V)

[88665-98-9]



M 459.0

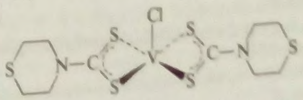
See also Chlorobis(4-thiomorpholinecarbodithioato-S^4,S^4) vanadium(*III*), IC-006972. Other thio-ligand vanadium complexes are also reported. Synth. by adding 2 moles of NaL to $VOCl_3$ in C_6H_6. Green solid.

Forghieri, F. *et al*, *Transition Met. Chem.*, 1983, **8**, 372 (*synth, uv-vis, ir*)

$C_{10}H_{16}ClN_2S_6V$ IC-006972

Chlorobis(4-thiomorpholinecarbodithioato-S^4,S^4) vanadium(*III*), 11Cl

[88665-91-2]



M 443.0

Synth. from VCl_3 and the Na salt of the ligand in MeOH. Yellow-green solid. Various related compds. also reported.

[65139-83-5]

Forghieri, F. *et al*, *Transition Met. Chem.*, 1983, **8**, 372 (*synth, uv-vis, ir*)

$C_{10}H_{10}Cl_4CrN_2$ IC-006973

Dichlorobis(3,5-dimethyl-1*H*-pyrazole-N^2)chromium(*III*), 9Cl

[59487-15-3]

$CrCl_2(C_5H_8N_2)_2$

M 315.1

Chloride-bridged polymer giving distorted octahedral coordination. Synth. from excess $CrCl_2$ + ligand in EtOH. Air-sensitive solid. Sol. DMF; insol. other common org. solvs. Ir $\nu_{C=N}$ 1260-1210, ν_{C-N} 110-295 cm^{-1}. μ_{eff} = 4.48μ_B (298K); 3.63μ_B (84K).

Mani, F. *et al*, *Inorg. Chim. Acta*, 1976, **16**, 163 (*synth, props*)

$C_{10}H_{10}Cl_2N_2OPt$ IC-006974

Dichloro(*N,N*-dimethylformamide-*O*)(2,6-dimethylpyridine)platinum(*II*), 10Cl

[70348-01-5]

An Dichloro(*N,N*-dimethylformamide-*O*)(pyridine)platinum(*II*), IC-005969 with

R = CH_3

M 446.2

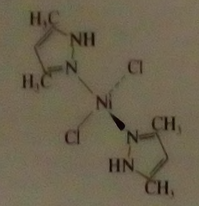
Square planar structure with *trans*-config. May form *cis*-config. in soln. Synth. from $Pt_2(Me_2Py)_2Cl_4$ + DMF. Yellow solid. Mp 160°.

Koog, P.-C. *et al*, *Can. J. Chem.*, 1979, **57**, 882 (*synth, ir*)
Rochon, F.D. *et al*, *Can. J. Chem.*, 1980, **58**, 97 (*struct*)

$C_{10}H_{10}Cl_2N_2Ni$ IC-006975

Dichlorobis(3,5-dimethyl-1*H*-pyrazole-N^2)nickel(*II*), 9Cl

[35592-96-2]



M 321.8

Probably tetrahedral. Pale-yellow cryst. Paramagnetic.

[63802-64-2]

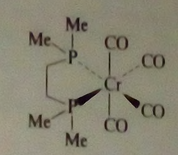
Nicholls, D. *et al*, *J. Inorg. Nucl. Chem.*, 1970, **32**, 3871 (*synth, uv, magnetism*)
Oglezneva, I.M. *et al*, *Zh. Neorg. Khim.*, 1985, **30**, 1473 (*ir*)

$C_{10}H_{16}CrO_4P_2$ IC-006976

Tetracarbonyl[1,2-ethanediylbis[dimethylphosphine]-*P,P*']chromium, 11Cl

Bis[1,2-bis(dimethylphosphino)ethane]tetracarbonylchromium

[40544-95-4]



M 314.1

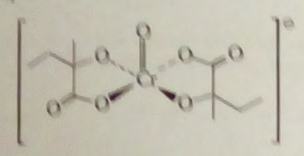
Octahedral. Pale yellow cryst. (EtOH at −45°). Mp 146-150°. Ir ν_{CO} 2009, 1921, 1900, 1894 cm^{-1} (hexane).

Connor, J.A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 347 (*synth, ir, pmr, PES*)
Grobe, J. *et al*, *Z. Naturforsch., B*, 1980, **35**, 533; 1981, **36**, 301, 482 (*synth*)
Cook, R.L. *et al*, *Inorg. Chem.*, 1984, **23**, 2332 (*ir, electrochem*)

$C_{10}H_{10}CrO_7^{\ominus}$ IC-006977

Bis[2-hydroxy-2-methylbutanoato(2−)-O^1,O^2] oxochromate(*V*)(1−), 11Cl, 10Cl

[59194-74-1]



M 300.2 (ion)

Many complexes of other α-hydroxycarboxylic acids also known. Salts sol. H_2O, Me_2CO etc., insol. non-polar solvs. Slow dec. to Cr(*III*) in H_2O. Heavy alkyl substitution stabilises hydroxy-carboxylate ligand to oxidation by Cr(*V*). Ph groups de-stabilise.

K salt: [94036-72-3].
First stable, well characterised Cr(*V*) complex of an α-hydroxycarboxylic acid. Dark brown cryst. + $1H_2O$ (Me_2CO/hexane). Sol. H_2O. Paramagnetic, μ_{eff} = 2.05μ_B. Ir $\nu_{C=O}$ 994 cm^{-1}.

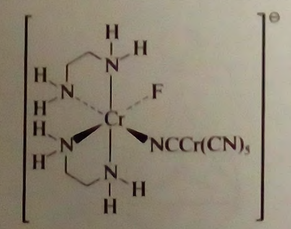
[65613-90-3]

Krumpolc, M. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 145; 1979, **101**, 3206 (*synth, cryst struct, uv, ir, esr*)
Inorg. Synth., 1982, **20**, 63 (*synth*)
Rajasekar, N. *et al*, *Inorg. Chem.*, 1983, **22**, 971.
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 936 (*rev*)
Ghosh, S.K. *et al*, *Inorg. Chem.*, 1988, **27**, 1620 (*kinetics*)

$C_{10}H_{16}Cr_2FN_{10}^{\ominus}$ IC-006978

μ-Cyanopentacyanobis(ethylenediamine) fluorodichromate(*III*)

[μ-(Cyano-C:N)]pentakis(cyano-C)bis(1,2-ethanediamine-N,N')fluorodichromate(III)(*1*−), *11Cl, 10Cl*



M 399.2 (ion)

Representative of many monocyano-bridged complexes; *cis*-octahedral.

Na salt: [75082-86-9].
Synth. by heating *trans*-$Na[CrF(en)_2H_2O][Cr(CN)_6]$.

K salt: [75058-06-9].
Synth. from aq. *trans*-$[CrF(H_2O)(en)_2](ClO_4)_2$ and $K_3Cr(CN)_6$. Pink solid (EtOH aq.). Antiferromagnetic.

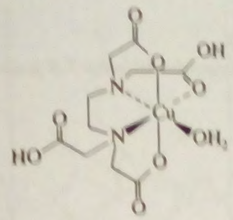
Ribas, J. *et al*, *Transition Met. Chem.*, 1984, **9**, 407 (*synth, uv, ir*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 777 (*rev*)

$C_{10}H_{10}CuN_2O_9$ IC-006979

Aqua(dihydrogen ethylenediaminetetraacetato)copper(*II*)

Aqua[(dihydrogen(ethylenedinitrilo)tetraacetato]copper(II), *8Cl*

[24778-06-1]



M 371.7

H_4edta acts as a quinquedentate ligand; octahedral at Cu.
Blue plates (aq. soln.).

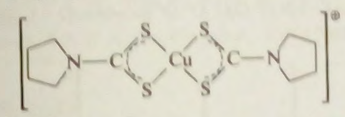
[26608-99-1]

Martynenko, L.I. *et al*, *Zh. Neorg. Khim.*, 1968, **13**, 2067 (*ir*)
Stephens, F.S., *J. Chem. Soc. A*, 1969, 1723 (*cryst struct*)
Hathaway, B.J. *et al*, *J. Chem. Soc. A*, 1969, 2312 (*uv, esr*)

$C_{10}H_{16}CuN_2S_4^{\oplus}$ IC-006980

Bis(1-pyrrolidinecarbodithioato-*S,S'*)copper(*III*)(1+), 10Cl

[23301-60-2]



M 356.0 (ion)

Square planar with formal Cu(*III*).

Perchlorate: [69951-83-3].
Cryst. ($CHCl_3$).
▷ Potentially explosive.

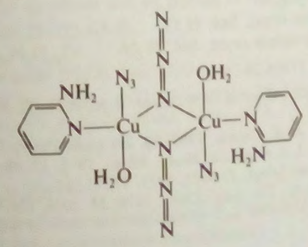
Chary, M.N. *et al*, *Indian J. Pure Appl. Phys.*, 1977, **15**, 172 (*esr*)
Herring, F.G. *et al*, *Can. J. Chem.*, 1979, **57**, 2379 (*synth, esr, ir*)
Brown, K.L. *et al*, *Cryst. Struct. Commun.*, 1979, **8**, 157 (*cryst struct*)

$C_{10}H_{16}Cu_2N_{10}O_2$ IC-006981

Diaquabis[μ-(azido-N^1:N^1)]diazidobis(2-pyridinamine-N^1) dicopper(*II*), 11Cl

Di-μ-azidobis[azido(2-aminopyridine)aquacopper(II)]

[91187-16-5]



M 519.4

Black cryst.

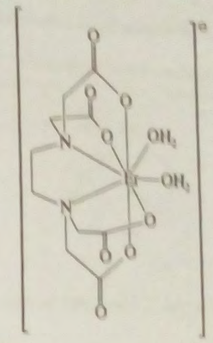
▷ $Cu(N_3)_2$, a by-product of the synth., is explosive.

Goher, M.A.S. *et al*, *Inorg. Chim. Acta*, 1984, **85**, 117 (*synth, cryst struct, ir, uv*)

$C_{10}H_{16}ErN_2O_{10}^{\ominus}$ IC-006982

Diaqua(ethylenediaminetetraacetato)erbate(*III*)(1−)

Diaqua[N,N'-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]] (*4*−)]*erbate*(*1*−)



M 491.5 (ion)

8-Coordinate.

K salt: [95821-40-5].
Pink cryst. Sol. H_2O.

NH_4 salt, trihydrate: [65805-08-5].
Pale rose-coloured plates. Sol. H_2O.

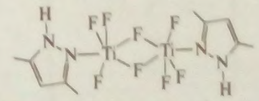
[101921-59-9]

Popov, K.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 725 (*synth*)
Filippova, T.V. *et al*, *Zh. Strukt. Khim.*, 1977, **18**, 1127 (*cryst struct*)

$C_{10}H_{16}F_8N_4Ti_2$ IC-006983

Bis(3,5-dimethyl-1*H*-pyrazole-N^2)di-μ-fluorohexafluorodititanium(*IV*), 11Cl

[101076-20-4]



M 440.0

Fluorine bridged dimer. The detailed arrangment is not known. Synth. by adding a CH_2Cl_2 soln. of the dimethylpyrazole to a slurry of TiF_4 in CH_2Cl_2.

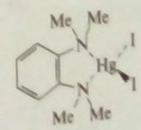
Perez, M.P.P. *et al*, *Acta Cient. Compostelana*, 1984, **21**, 27; *CA*, **104**, 140938c (*synth, ir, raman*)

$C_{10}H_{16}HgI_2N_2$ IC-006984

Diiodo(*N,N,N',N'*-tetramethyl-1,2-benzenediamine-N,N') mercury(*II*), 11Cl

Diiodo(N,N,N',N'-*tetramethyl-1,2-diaminobenzene*)*mercury*

[15629-72-8]



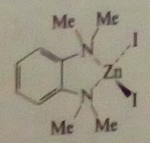
M 618.6

Tetrahedral at Hg. Cryst. Mp 165° dec. Dichloro and dibromo analogues are known.

Sindellari, L., *Ann. Chim. (Rome)*, 1966, **56**, 386 (*synth, str*)
Hughes, C.M. *et al, Aust. J. Chem.*, 1985, **38**, 1521 (*synth, cryst struct*)

IC-006985

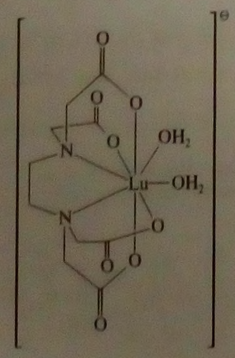
$C_{10}H_{16}I_2N_2Zn$
Diiodo(*N,N,N′,N′*-tetramethyl-1,2-benzenediamine-*N,N′*)zinc, 11Cl
[1,2-Bis(dimethyldiamino)benzene]diiodozinc
[99394-09-9]



M 483.4
Cryst.
Hughes, C.M. *et al, Aust. J. Chem.*, 1985, **38**, 1521 (*synth, cryst struct*)

IC-006986

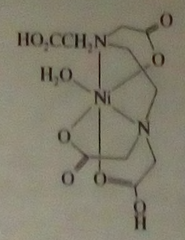
$C_{10}H_{16}LuN_2O_{10}^{\ominus}$
Diaqua(ethylenediaminetetraacetato)lutetate(*III*)(1−)
Diaqua[[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]]*(4−)*]*lutetate(1−), 11Cl*
[98521-56-3]



M 499.2 (ion)
8-Coordinate.
K salt: [98521-42-7].
Colourless cryst. Sol. H_2O.
Ternovaya, T.V. *et al, Teor. Eksp. Khim.*, 1985, **21**, 440; *CA*, **104**, 14001 (*ir, nmr, tga*)

IC-006987

$C_{10}H_{16}N_2NiO_9$
Aqua(dihydrogen ethylenediaminetetraacetato)nickel(*II*)
Aqua[ethylenediamine(diacetic acid)diacetato]nickel(II).
Dihydrogen ethylenediaminetetraacetatoaquanickel(II)

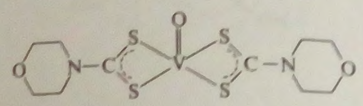


M 366.9

Octahedral at Ni, exact position of hydroxy H uncertain. Prepd. from the ligand and Ni salts or $Ni(OH)_2$. Bright blue prismatic rods.
Brintzinger, H. *et al, Z. Anorg. Allg. Chem.*, 1942, **249**, 113 (*synth*)
Smith, G.S. *et al, J. Am. Chem. Soc.*, 1959, **81**, 556 (*synth, cryst struct*)

IC-006988

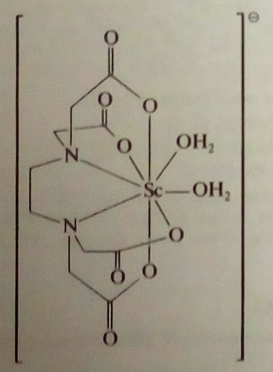
$C_{10}H_{16}N_2O_3S_4V$
Bis(4-morpholinecarbodithioato-*S,S′*)oxovanadium(*IV*), 11Cl
[33873-75-5]



M 391.4
Synth. by adding the ligand in EtOH to aq. $VOSO_4$ or from NaL + $VOSO_4$. Grey-green solid. Paramagnetic, $\mu_{eff} = 1.69\mu_B$(301K).
Dey, K. *et al, Indian J. Chem., Sect. A*, 1977, **15**, 49 (*synth, magnetism*)
Forghieri, F. *et al, Transition Met. Chem.*, 1983, **8**, 372 (*synth, ir, uv-vis*)

IC-006989

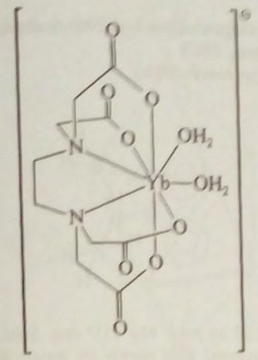
$C_{10}H_{16}N_2O_{10}Sc^{\ominus}$
Diaqua(ethylenediaminetetraacetato)scandate(*III*)(1−)
Diaqua[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*(4−)-N,N′,O,O′,O″,O‴]]*scandate(1−), 10Cl*
[67816-27-7]



M 369.2 (ion)
H compd.: [12611-55-1].
$C_{10}H_{17}N_2O_{10}Sc$ M 370.2
Colourless cryst. Sol. H_2O.
K salt: Colourless cryst. Sol. H_2O.
[12611-55-1, 17595-28-7]
Schwarzenbach, G. *et al, Helv. Chim. Acta*, 1954, **37**, 937 (*stability consts*)
Merbach, A. *et al, Chimia*, 1969, **23**, 271 (*synth, pmr*)
Martynenko, L.I. *et al, Zh. Neorg. Khim.*, 1971, **17**, 98; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **17**, 51 (*ir*)
Amsheeva, A.A., *Zh. Anal. Khim.*, 1978, **33**, 1054; *CA*, **89**, 190275 (*synth*)

IC-006990

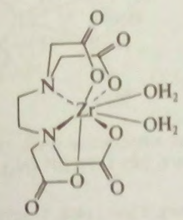
$C_{10}H_{16}N_2O_{10}Yb^{\ominus}$
Diaqua(ethylenediaminetetraacetato)ytterbate(*III*)(1−)
Triaqua[[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*](4−)]]*ytterbate(1−), 9Cl*
[98575-90-7]



M 497.2 (ion)
8-Coordinate.
K salt: [98575-89-4].
Colourless cryst. Sol. H_2O.
Cs salt: [70948-72-0].
Colourless cryst. $+3H_2O$. Sol. H_2O.
Popov, K.I. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 725 (*synth*)
Nassimbeni, L.R. *et al, Acta Crystallogr., Sect. B*, 1979, **35**, 1341 (*cryst struct*)

IC-006991

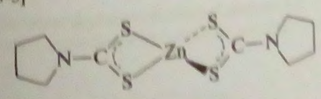
$C_{10}H_{16}N_2O_{10}Zr$
Diaqua(ethylenediaminetetraacetato)zirconium(*IV*)
Diaqua[[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](4-)-N,N′,O,O′,O^N,O^N]*zirconium, 9Cl*
[98575-90-7]



M 415.4
8-Coordinate distorted dodecahedron. Synth. from $ZrCl_4$ and the disodium salt of EDTA in hot water.
Dihydrate: [51321-09-6].
$C_{10}H_{20}N_2O_{12}Zr$ M 451.4
White solid (H_2O). Sol. H_2O.
Langer, H.G., *J. Inorg. Nucl. Chem.*, 1964, **26**, 59 (*synth, ir*)
Pozhidaev, A.I. *et al, Zh. Strukt. Khim.*, 1973, **14**, 947; 1974, **15**, 644 (*cryst struct*)

IC-006992

$C_{10}H_{16}N_2S_4Zn$
Bis(1-pyrrolidinecarbodithioato-*S,S′*)zinc(*II*), 9Cl
Zinc(II) *bis(1-pyrrolidinecarbodithioate)*
[40211-68-5]

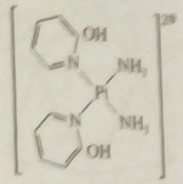


M 357.9

Solid. $Bp_{0.015-0.03}$ 176°.
Schaefe, F.R. *et al, Anal. Chem.*, 1970, **42**, 613 (*stability consts*)
Malissa, H. *et al, Anal. Chim. Acta*, 1973, **63**, 225 (*ir*)
Kellner, R., *Anal. Chim. Acta*, 1973, **66**, 49 (*ir*)
Dias, J.R. *et al, Org. Mass Spectrom.*, 1981, **16**, 12 (*ms*)
Meula-Zigon, M. *et al, CA*, 1982, **96**, 209818 (*synth, ms, pmr*)

IC-006993

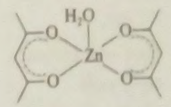
$C_{10}H_{16}N_4O_2Pt^{2\oplus}$
Diamminebis(2-hydroxypyridine-*N*)platinum(*II*)(2+)
Diamminebis(2-pyridinol)platinum(2+), 10Cl
Diamminebis(2-pyridone)platinum(II)



M 419.3 (ion)
Minor product of reaction producing pyridonato complex.
cis-form
Dichloride: [76761-67-6].
$C_{10}H_{16}Cl_2N_4O_2Pt$ M 490.2
White cryst. Sol. H_2O.
Hollis, L.S. *et al, Inorg. Chem.*, 1983, **22**, 2708 (*synth, struct*)

IC-006994

$C_{10}H_{16}O_5Zn$
Aquabis(2,4-pentanedionato-*O,O′*)zinc, 9Cl
Bis(2,4-pentanedionato)aquazinc. Bis(acetylacetonato) aquazinc
[35827-32-8]



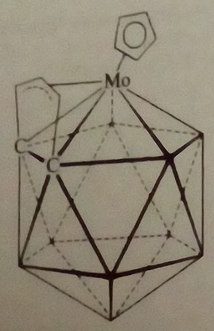
M 281.6
Monomeric in solid state. Coordination of Zn intermed. between tetragonal pyramidal and trigonal bipyramidal. Commercially available. Used in coupling of organoboranes. Needles (C_6H_6, EtOH or C_6H_6/EtOH). Mp 138°. Not v. stable in air; hydrol. by H_2O; dec. slowly above 60°; dec. at 130° to give mesitylene and $OAc^{\ominus}$. Dehydrates *in vacuo* over P_2O_5 to Bis(2,4-pentanedionato-*O,O′*)zinc, IC-006935.
Montgomery, H. *et al, Acta Crystallogr.*, 1963, **16**, 748 (*cryst struct*)
Graddon, D.P. *et al, Aust. J. Chem.*, 1963, **16**, 980 (*synth*)
Rudolph, G. *et al, Inorg. Chem.*, 1964, **3**, 1317 (*thermoch*)
Nakamura, Y. *et al, Inorg. Chem.*, 1975, **14**, 63 (*ir*)
Takegoshi, K. *et al, Inorg. Chem.*, 1987, **26**, 2552 (*solid state cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 33 (*use*)

$C_{10}H_{17}B_9Mo$ IC-006995

1-η^5-Cyclopentadienylmolybdenum-η^3:η^2-allyla-2,3-dicarbaborane(9)

(η^5-2,4-Cyclopentadien-1-yl)[η^3-1,2,3,4,5,6,9,10,11-nonahydro-7,8-(1-propene-1,3-diyl)-7,8-dicarbaundecaborato(3−)]molybdenum, 12CI

[126883-29-2]



M 330.4

Air-stable solid. Sol. Et_2O, toluene.

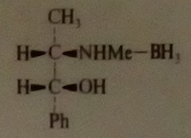
Grebenik, P.D. *et al*, *J. Chem. Soc., Chem. Commun.*, 1989, 1397 (*synth, pmr, B-11 nmr, cmr, cryst struct*)

$C_{10}H_{18}BNO$ IC-006996

(Ephedrine)trihydroboron

Borane ephedrine. Trihydro[α-[1-(methylamino)ethyl]benzenemethanol-N]boron, 10CI. α-[1-(Methylamino)ethyl]benzenemethanol compd. with borane (1:1). 1,N-Dimethyl-2-hydroxy-2-phenylethylamine borane

[73798-15-9]



M 179.0

Chiral reducing complex.

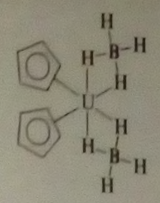
Johnson, C.R. *et al*, *Tetrahedron Lett.*, 1979, 4713.
Grundon, M.F. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1981, 231 (*synth*)
Mancilla, T. *et al*, *Tetrahedron Lett.*, 1982, **23**, 1561 (*ir, raman, nmr*)

$C_{10}H_{18}B_2U$ IC-006997

Bis(η^5-2,4-cyclopentadien-1-yl)bis[tetrahydroborato(1−)-*H*,*H*']uranium, 10CI

Bis(cyclopentadienyl)uranium bis(tetrahydroborate)

[65888-45-1]



M 397.9

V. oxygen- and moisture-sensitive red-brown solid. Sol. THF, dimethoxyethane. Subl. 60° *in vacuo*.

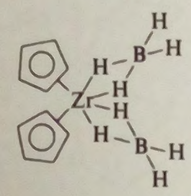
Zanella, P. *et al*, *J. Organomet. Chem.*, 1977, **142**, C21 (*synth, struct, ir, nmr*)

$C_{10}H_{18}B_2Zr$ IC-006998

Bis(η^5-2,4-cyclopentadien-1-yl)bis[tetrahydroborato(1−)-*H*,*H*']zirconium, 10CI

Zirconocene bis(borohydride)

[12083-77-1]



M 251.0

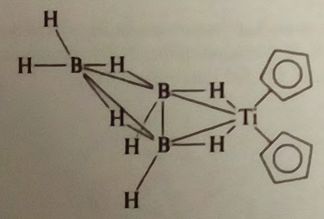
Pale-yellow solid by subl. Mp 155° dec. Subl. 110-115° *in vacuo*. Hydrolysed only slowly by water. BD_4 analogue also made.

Nanda, R.K. *et al*, *Inorg. Chem.*, 1964, **3**, 1798 (*synth, ir*)
Davies, N. *et al*, *J. Chem. Soc. A*, 1969, 2601 (*ir, nmr*)
Marks, T.J. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 3397 (*ir, nmr*)
Smith, B.E. *et al*, *J. Inorg. Nucl. Chem.*, 1976, **38**, 1973 (*synth, ir, raman*)

$C_{10}H_{18}B_3Ti$ IC-006999

Bis(η^5-2,4-cyclopentadien-1-yl)[octahydroborato(1−)-H^1,H^3]titanium

Di-π-cyclopentadienyl[octahydrotriborato(1−)]titanium, 8CI



M 218.5

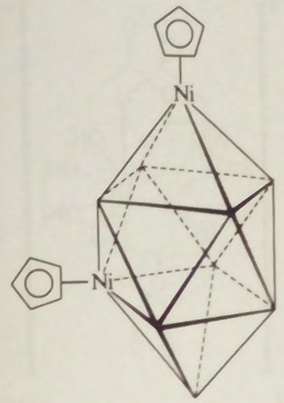
arachno-. Dark blue air-sensitive cryst. (by subl.). Sol. non-polar solvs., ethers. Mp 117-120° (N_2). $Subl._{0.001}$ 120-150°.

Klanberg, F. *et al*, *Inorg. Chem.*, 1968, **7**, 2272 (*synth, props, ms, ir, deriv*)

$C_{10}H_{18}B_8Ni_2$ IC-007000

Bis(η^5-2,4-cyclopentadien-1-yl)[μ-[η^4:η^5-octahydrooctaborato(2−)]]dinickel, 10CI

[72098-83-0]



M 342.1

closo-. Synth. from NaB_5H_8 + NaC_5H_5 + $NiBr_2$ in cold THF. Orange solid.

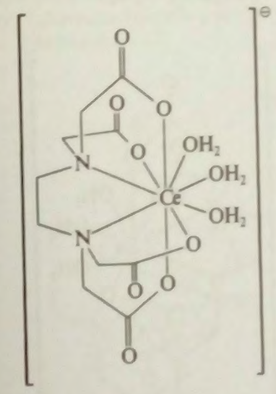
Grimes, R.N. *et al*, *J. Am. Chem. Soc.*, 1979, **101**, 6229 (*synth, B-11 nmr, pmr, ir*)

$C_{10}H_{18}CeN_2O_{11}^{\ominus}$ IC-007001

Triaqua(ethylenediaminetetraacetato)cerate(*III*)(1−)

Triaqua[[N,N'-1,2-ethanediylbis[N-(carboxymethyl)glycinato]](4−)-N,N',O,O',O'',O''']cerate(1−), 9CI

[98521-47-2]



M 482.3 (ion)

Presumed 9-coordinate as shown.

Na salt: Colourless cryst. + $5H_2O$. Sol. H_2O. μ_{eff} = $2.37\mu_B$. Dec. at 235°.

K salt: [98521-35-8].

Cryst. Sol. H_2O.

Kusakina, N.P. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1965, **10**, 547 (*synth, ir, tga, magnetism*)
Ternovaya, T.V. *et al*, *Teor. Eksp. Khim.*, 1985, **21**, 440 (*ir, tga, uv-vis*)

$C_{10}H_{18}Cl_2N_2Pt$ IC-007002

Dichlorobis(trimethylacetonitrile)platinum(*II*)

Dichlorobis(2,2-dimethylpropanenitrile)platinum, 9CI

[51014-04-1]

$[(H_3C)_3CCN]_2PtCl_2$

M 432.2

Despite its use in synth. clear details of its preparation and characterisation are not available. The appropriate isomer can probably be obtained by suitable application of the *trans*-effect. Useful starting materials for other Pt complexes.

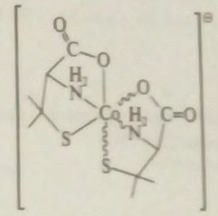
[41884-65-5, 60479-35-8]

Mason, R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 297.
Moulton, C.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1976, 365.

$C_{10}H_{18}CoN_2O_4S_2^{\ominus}$ IC-007003

Bis(D-pencillaminato)cobaltate(*III*)(1−)

Bis[3-mercapto-D-valinato(2−)-N,O,S']cobaltate(III)(1−), 11CI



M 353.3 (ion)

Stereochem. not established.

K salt: [63016-35-3].

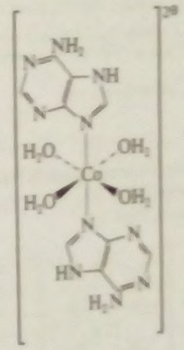
Brown needles + $2H_2O$. Sol. H_2O.

Okomato, W. *et al*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 165 (*synth, str*)

$C_{10}H_{18}CoN_{10}O_4^{2\oplus}$ IC-007004

Bis(adenine)tetraaquacobalt(*II*)(2+)

Tetraaquabis(9H-purin-6-amine-N^7)cobalt(2+), 9CI



M 401.2 (ion)

trans-Octahedral struct.

Bis(hydrogen sulfate): [50284-21-4].

Pink needles + adenine + $6H_2O$.

de Meester, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1596 (*synth, cryst struct*)

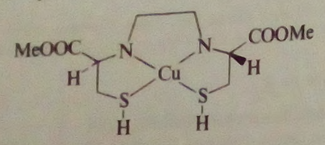
IC-007005

$C_{10}H_{18}CuN_2O_4S_2$

[[Dimethyl *N,N'*-1,2-ethanediylbis[L-cysteinato]](2−)-*N,N',S,S'*]copper(*II*), 11CI

[Dimethyl N,N'*-ethylenebis(*L*-cysteinato)(2−)-S,S']copper*(II)

[101032-89-7]



M 357.9

Square planar Cu. Red-brown plates.

Bharadwaj, P.K. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 1351 (*synth, cryst struct*)

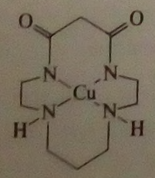
IC-007006

$C_{10}H_{18}CuN_4O_2$

[1,4,8,11-Tetraazacyclotetradecane-5,7-dionato(2−)-N^1,N^4,N^8,N^{11}]copper(*II*), 11CI

(Dioxocyclam)copper(II)

[72547-88-7]



M 289.8

Pink-violet cryst. + $2H_2O$ (EtOH). Stable over large pH range. Easily oxidised to related Cu(*III*) complex. Mod. sol. H_2O, sl. sol. MeOH, EtOH, insol. most org. solvs.

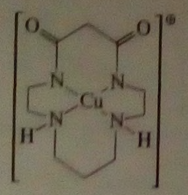
Kodama, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 325 (*synth*)
Fabbrizi, L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1980, 646 (*electrochem*)
Inorg. Synth., 1985, **23**, 82 (*synth, vis*)

IC-007007

$C_{10}H_{18}CuN_4O_2^{\oplus}$

[1,4,8,11-Tetraazacyclotetradecane-5,7-dionato(2−)-N^1,N^4,N^8,N^{11}]copper(*III*)(1+)

(Dioxocyclam)copper(III)(*1+*)



M 289.8 (ion)

Synth. from [1,4,8,11-Tetraazacyclotetradecane-5,7-dionato(2−)-N^1,N^4,N^8,N^{11}]copper(*II*), IC-007006 by reaction with $K_2S_2O_8$ in H_2O, or by controlled potential electrolysis. Example of a Cu(*III*) complex stabilised by macrocyclic ligand. Yellow brown; stable in soln. for 2-3 h. Sol. H_2O. E° $[Cu^{III}(dioxocyclamato(2-))]^{\oplus}/[Cu^{II}(dioxocyclamato(2-))] = 0.88V$ vs SHE.

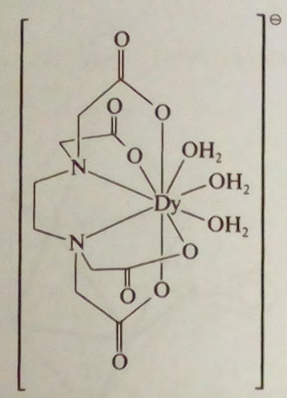
Kodama, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 325; 1981, 694 (*synth, electrochem*)
Fabbrizi, L. *et al*, *J. Chem. Soc., Chem. Commun.*, 1980, 646 (*electrochem*)
Inorg. Synth., 1985, **23**, 82 (*synth*)

IC-007008

$C_{10}H_{18}DyN_2O_{11}^{\ominus}$

Triaqua(ethylenediaminetetraacetato)dysprosate(*III*)(1−)

Triaqua[[N,N'*-1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4−*)]*dysprosate*(*1−*), *9CI*



M 504.7 (ion)

9-Coordinate.

Na salt: [71229-12-4].
Yellow cryst. + $5H_2O$. Sol. H_2O.

Popov, K.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 725 (*synth*)
Nassimbeni, L.R. *et al*, *Acta Crystallogr., Sect. B*, 1979, **35**, 1341 (*cryst struct*)

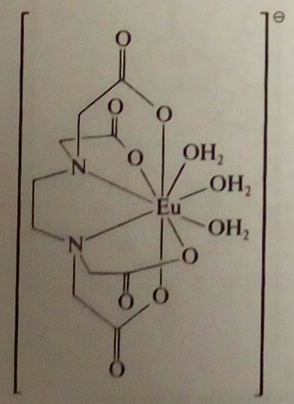
IC-007009

$C_{10}H_{18}EuN_2O_{11}^{\ominus}$

Triaqua(ethylenediaminetetraacetato)europate(*III*)(1−)

Triaqua[[N,N'*-1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4−*)]*europate*(*1−*), *9CI*

[76147-55-2]



M 494.2 (ion)

Assumed 9-coordinate.

Na salt: [41742-73-8].
Colourless cryst. + $5H_2O$. Sol. H_2O.

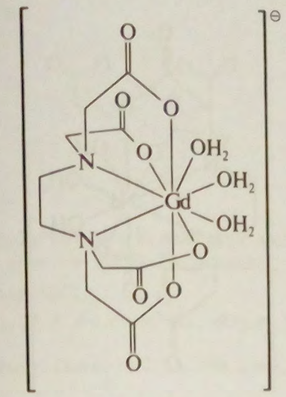
Bredenfel'd, N.V. *et al*, *Russ. J. Phys. Chem. (Engl. Transl.)*, 1970, **44**, 1544 (*synth, fluorescence*)
Popov, K.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 725 (*synth*)

IC-007010

$C_{10}H_{18}GdN_2O_{11}^{\ominus}$

Triaqua(ethylenediaminetetraacetato)gadolinate(*III*)(1−)

Triaqua[[N,N'*-1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4−*)]*gadolinate*(*1−*), *11CI*



M 499.5 (ion)

9-Coordinate.

Na salt: [83486-29-7].
White cryst. + $5H_2O$. Sol. H_2O.

K salt: White cryst. + $5H_2O$. Sol. H_2O.

Moeller, T. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 3182 (*synth, ir*)
Fritz, J.J. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 6199 (*magnetism*)
Fritz, J.J. *et al*, *J. Phys. Chem.*, 1961, **65**, 2070 (*magnetism*)
Templeton, L.K. *et al*, *Acta Crystallogr., Sect. B*, 1982, **38**, 2155 (*cryst struct*)

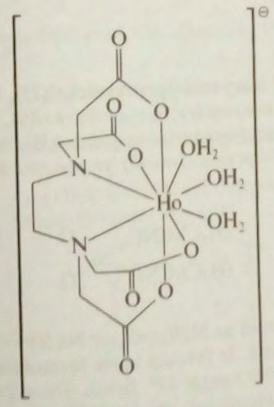
IC-007011

$C_{10}H_{18}HoN_2O_{11}^{\ominus}$

Triaqua(ethylenediaminetetraacetato)holmate(*III*)(1−)

Triaqua[N,N'*-1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*(*4−*)]]*holmate*(*1−*)

[76147-52-9]



M 507.1 (ion)

9-Coordinate Ho.

Na salt: [95718-59-5].
Yellow cryst. + $5H_2O$. Sol. H_2O.

Alsaadi, B.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 2151 (*synth, pmr*)
Templeton, L.K. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 355 (*synth, cryst struct*)

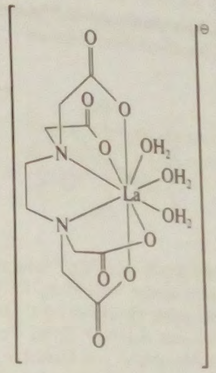
IC-007012

$C_{10}H_{18}LaN_2O_{11}^{\ominus}$

Triaqua(ethylenediaminetetraacetato)lanthanate(*III*)(1−)

Triaqua[[N,N'*-1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4−*)-N,N',O,O'O^8,O^8']*lanthanate*(*1−*), *9CI*

[21647-53-0]



M 481.1 (ion)

9-Coordinate.

Na salt: [29258-37-5].
Colourless cryst. + $5H_2O$. Sol. H_2O.

K salt: [19663-24-2].
Colourless cryst. + $5H_2O$. Sol. H_2O.

H compd.: see *Tetraaqua*[[N,N'*-1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*3−*)-N,N',O,O',O^8,O^8']*lanthanum*(III), *IC-007102*

[51406-94-1]

Hoard, J.L. *et al*, *J. Am. Chem. Soc.*, 1965, **87**, 1612 (*synth, cryst struct*)
Martynenko, L.I. *et al*, *Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 725 (*synth*)
Djordjevic, C. *et al*, *Inorg. Chem.*, 1980, **19**, 3049 (*synth*)
Djordjevic, C. *et al*, *J. Less-Common Met.*, 1983, **94**, 355 (*pmr, cmr*)

IC-007013

$C_{10}H_{18}MnN_2O_4S_2^{2\ominus}$

Bis[penicillaminato(2−)]manganate(*II*)(2−)

Bis[*3-mercapto-D-valinato*(2−)-N,S]*manganate*(2−), *11CI*

$Mn[OOCCH(NH_2)C(CH_3)_2S]_2^{2\ominus}$

M 349.3 (ion)

Struct. not known.

Di-Na salt: Synth. in aq. soln. Green. Forms adduct with O_2 reversibly at r.t. which catalyses oxidative extradiol cleavage of pyrocatechol.

[87792-91-4]

Doornbos, D.A., *Pharm. Weekbl.*, 1968, **103**, 1213 (*exhibits convuls*)
Sakurai, H., *Biochem. Biophys. Res. Commun.*, 1983, **115**, 618 (*uv, vis, esr, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 292 (*text, bibl*)

IC-007014

$C_{10}H_{18}MnO_4$

Manganese bis(trimethylacetate)

Dipivalatomanganese(II). *Manganese dipivalate. Bis(2,2-dimethylpropanoato)manganese*(II)

$Mn[OOCC(CH_3)_3]_2$

M 257.1

Struct. not known. Prepd. from $MnCl_2$ and potassium pivalate under Ar. Dec. in air to form $[Mn_3^{III}O(OOCCMe_3)_6][Me_3CCO_2]$

Pasynskii, A.A. *et al, Sov. J. Coord. Chem. (Engl. Transl.)*, 1976, **2**, 813 (*synth, props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 68 (*rev, bibl*)

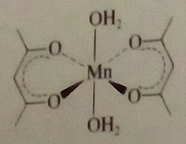
IC-007015

$C_{10}H_{18}MnO_6$

Diaquabis(2,4-pentanedionato-*O,O'*)manganese(*II*), 11CI

Manganese(II) *acetoacetonate dihydrate*

[14024-80-7]



M 289.1
trans-Octahedral. Synth. from $Mn^{2\oplus}$ salts and 2,4-pentanedione in acetate buffered aq. EtOH. Air-sensitive, pale-yellow pleochroic cryst. Forms $Mn(acac)_2$ on heating *in vacuo*. Sol. H_2O, EtOH, Py; insol. Et_2O. In alkaline soln. $Mn(acac)_3^{\ominus}$ ions formed. $\mu_{eff} = 6.02\mu_B$ (292K). H_2O ligands readily replaced by O and N donor ligands.

Inorg. Synth., 1960, **6**, 164 (*synth*)
Holm, R.H. *et al, J. Phys. Chem.*, 1961, **65**, 321 (*esr*)
Graddon, D.P. *et al, Aust. J. Chem.*, 1964, **17**, 1119 (*magnetism*)
Dingle, R., *Acta Chem. Scand.*, 1966, **20**, 33 (*uv*)
Montgomery, H. *et al, Acta Crystallogr., Sect. B*, 1968, **24**, 1127 (*cryst struct*)
Onuma, S. *et al, Bull. Chem. Soc. Jpn.*, 1970, **43**, 2395 (*cryst struct*)
Das, A.K. *et al, Curr. Sci.*, 1970, **39**, 60 (*ir*)
Matsushita, T. *et al, CA*, 1974, **81**, 144920 (*ir*)
O'Connor, C.J. *et al, Inorg. Chem.*, 1975, **14**, 291 (*props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 71 (*rev, bibl*)

IC-007016

$C_{10}H_{18}MnO_6^{\ominus}$

Diaquabis(2,4-pentanedionato-*O,O'*)manganese(*III*)(1+), 11CI

Bis(acetylacetonato)diaquamanganese(III)(*1+*)

[82931-96-2]

$[Mn(OH_2)_2(acac)_2]^{\oplus}$

M 289.1 (ion)
Geometry not known.
Chloride: Synth. from $Mn(acac)_3$ and HCl or from $MnCl_2$, $KMnO_4$ + acacH in H_2O. Dark green cryst. + $2H_2O$. Dec. in H_2O to give $Mn_2O_3.xH_2O$.
Perchlorate: Synth. from $Mn(acac)_3$ and $HClO_4$. Dark green cryst. + $2.5H_2O$. Dec. in H_2O to give $Mn_2O_3.xH_2O$.
▷ Potentially explosive.

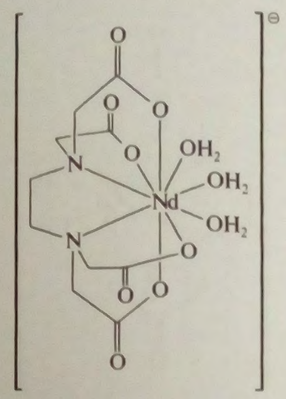
Cartledge, G.H., *J. Am. Chem. Soc.*, 1952, **74**, 6015 (*synth, uv*)
Davis, T.S. *et al, Inorg. Chem.*, 1968, **7**, 1994 (*uv*)
Isobe, K. *et al, Inorg. Nucl. Chem. Lett.*, 1973, **9**, 1283 (*synth*)
Isobe, K. *et al, Bull. Chem. Soc. Jpn.*, 1975, **48**, 250 (*synth, ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1979, **D1**, 98 (*rev, bibl*)

IC-007017

$C_{10}H_{18}N_2NdO_{11}^{\ominus}$

Triaqua(ethylenediaminetetraacetato)neodymate(*III*)(1–)

Triaqua[[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4–*)]*neodymate*(*1–*), *9CI*



M 486.4 (ion)
9-Coordinate.
Li salt: Purple cryst. + H_2O. Sol. H_2O.
Na salt: [17856-19-8].
Purple cryst. + $5H_2O$. Sol. H_2O.
K salt: [17856-18-7].
Purple cryst. + $5H_2O$. Sol. H_2O.
Rb salt: Purple cryst. + $2H_2O$. Sol. H_2O.
Cs salt: [60004-15-1].
Purple cryst. + H_2O. Sol. H_2O.
NH_4 salt: Purple cryst. + $5H_2O$. Sol. H_2O.

Moeller, T. *et al, J. Am. Chem. Soc.*, 1955, **77**, 3182 (*synth*)
Hoard, J.L. *et al, J. Am. Chem. Soc.*, 1965, **87**, 1612 (*struct*)
Charles, R.G., *J. Inorg. Nucl. Chem.*, 1966, **28**, 407 (*synth, props*)
Popov, K.I. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1975, 1710; 1976, 708 (*pmr*)
Matkovic-Calogovic, D., *Acta Crystallogr., Sect. C*, 1988, **44**, 435 (*cryst struct*)

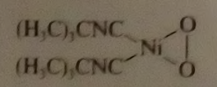
IC-007018

$C_{10}H_{18}N_2NiO_2$

Bis(*tert*-butyl isocyanide)peroxynickel(*II*), 8CI

Bis(tert-*butyl isocyanide*)(*dioxygen*)*nickel*(*0*), *8CI*. *Bis*(*2-isocyano-2-methylpropane*)*peroxynickel*(II), *9CI*. *Dioxygenbis*(*2-isocyano-2-methylpropane*)*nickel*(*0*), *9CI*

[19633-19-3]



M 256.9
Can be considered as Ni(0)—O_2 or Ni(*II*)—$O_2^{2\ominus}$ complex, or intermediate. Ir favours latter formulation. O_2 bidentate, ONiO angle 47°. Synth. from Tetrakis(*tert*-butylisocyanide)nickel, IC-010713 + O_2 in Et_2O at −20°. Undergoes oxidising reactions, or loses O_2. Pale green prisms (toluene). Sol. $CHCl_3$, toluene, $C_6H_5CF_3$.
▷ Dry samples may explode.

[24981-96-2, 32824-82-1, 34902-28-8]

Otsuka, S. *et al, J. Am. Chem. Soc.*, 1969, **91**, 6994 (*synth, ir, raman*)
Matsumoto, M. *et al, Acta Crystallogr., Sect. B*, 1975, **31**, 2711 (*cryst struct*)
Arzoumanian, H. *et al, J. Organomet. Chem.*, 1984, **267**, 207 (*reaction*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **6**, 329 (*reactions*)

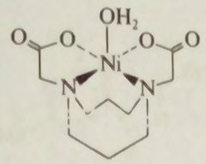
IC-007019

$C_{10}H_{18}N_2NiO_5$

Aqua(1,5-diazacyclooctane-*N,N'*-diacetato)nickel(*II*)

Aqua[*tetrahydro-1,5-diazocine-1,5-*(2H,6H)-*diacetato*(*2–*)-N^1,N^5,O^1,O^5]*nickel*, *9CI*

[56604-45-6]



M 304.9
Square-pyramidal complex in solid state and aq. soln. Blue-green cryst. + $2H_2O$. Paramagnetic.

[21485-30-3, 39034-58-7]

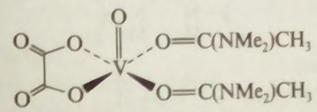
Nielson, D.O. *et al, J. Am. Chem. Soc.*, 1971, **93**, 5079 (*cryst struct*)
Averill, D.F., *Inorg. Chem.*, 1972, **11**, 2344 (*synth, ir, uv, struct, magnetism*)
Campbell, L. *et al, Inorg. Chem.*, 1978, **17**, 3378 (*props*)
Billo, E.J., *Inorg. Chim. Acta*, 1979, **37**, L533 (*props*)

IC-007020

$C_{10}H_{18}N_2O_7V$

Bis(*N,N*-dimethylacetamide-*O*)[ethanedioato(2–)-*O,O'*]oxovanadium(*IV*), 11CI

[55189-61-2]



M 329.2
Square pyramidal. Synth. by adding saturated aq. $VO(C_2O_4)$ to dimethylacetamide in Me_2CO. Blue solid.

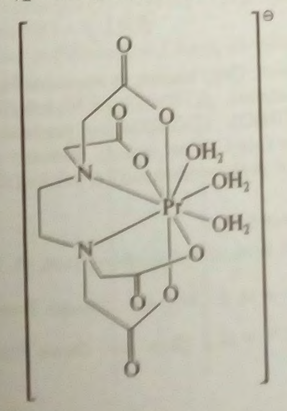
Durgaprasad, G. *et al, Indian J. Chem.*, 1974, **12**, 840 (*synth, uv-vis, ir*)
Usmankhodzhaeva, Ya.S. *et al, Uzb. Khim. Zh.*, 1983, 3; *CA*, **98**, 209087b (*synth, ir*)

IC-007021

$C_{10}H_{18}N_2O_{11}Pr^{\ominus}$

Triaqua(ethylenediaminetetraacetato)praseodymate(*III*)(1–)

Triaqua[[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4–*)]*praseodymate*(*1–*), *9CI*



M 483.1 (ion)
9-Coordinate.
Na salt: [82934-26-7].
Green cryst. + $5H_2O$. Sol. H_2O.

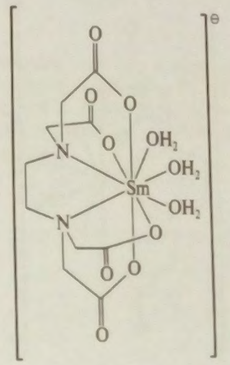
IC-007022

$C_{10}H_{18}N_2O_{11}Sm^{\ominus}$

Triaqua(ethylenediaminetetraacetato)samarate(*III*)(1–)

Triaqua[[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4–*)]*samarate*(*1–*), *9CI*

[76147-56-3]



M 492.6 (ion)
9-Coordinate.
Na salt: [58894-98-7].
Yellow cryst. + $5H_2O$. Sol. H_2O.

Moeller, T., *J. Am. Chem. Soc.*, 1955, **77**, 3182 (*synth*)
Fritz, J.J. *et al, J. Am. Chem. Soc.*, 1960, **82**, 6199 (*magnetism*)
Fritz, J.J. *et al, J. Phys. Chem.*, 1961, **65**, 2070.
Popov, K.I. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1976, 725.
Templeton, L.K. *et al, Acta Crystallogr., Sect. B*, 1982, **38**, 2155 (*cryst struct*)

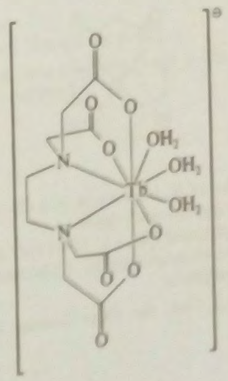
IC-007023

$C_{10}H_{18}N_2O_{11}Tb^{\ominus}$

Triaqua(ethylenediaminetetraacetato)terbate(*III*)(1–)

Triaqua[[N,N′-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](*4–*)]*terbate*(*1–*)

[76147-54-1]



M 501.1 (ion)
9-Coordinate.
Na salt: [56398-52-8].

Pink cryst. + $5H_2O$. Sol. H_2O. Isostruct. with others in series.

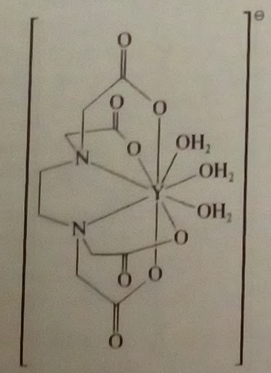
K salt: Pink cryst. Sol. H_2O.

Lee, B., *Diss. Abstr. B*, 1967, **28**, 84 (*cryst struct*)
Neelakantan, K. *et al*, *Inorg. Nucl. Chem. Lett.*, 1974, **10**, 67 (*kinetics*)
Gmelin Handbook Inorg. Chem., Syst. No. 39, 1980, **D1**, 177 (*struct*)
Ternovaya, T.V. *et al*, *Teor. Eksp. Khim.*, 1985, **21**, 440; *CA*, 1986, **104**, 14001 (*ir, tga, uv-vis*)

$C_{10}H_{18}N_2O_{11}Y^{\ominus}$ IC-007024

Triaqua(ethylenediaminetetraacetato)yttrate(*III*)(1−)

Triaqua[N,N′-*1,2-Ethanediylbis*[N-(*carboxymethyl*)*glycinato*(4−)-N,N′,O,O′,O″,O‴]]*yttrate*(1−)



M 431.1 (ion)
9-Coordinate.

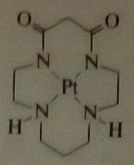
Na salt: Colourless cryst. + $5H_2O$. Sol. H_2O. Similar compds. obt. with other alkali metals.
Ca salt (2:1): Hygroscopic white cryst. + $4H_2O$. Sol. H_2O.
Sr salt (2:1): Hygroscopic white cryst. + $4H_2O$. Sol. H_2O.

Marsh, J.K., *J. Chem. Soc.*, 1950, 1819; 1955, 451 (*synth, props*)
Moeller, T. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 3182 (*synth, ir*)
Tananaev, I.V. *et al*, *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1963, **8**, 271 (*synth*)

$C_{10}H_{18}N_4O_2Pt$ IC-007025

[1,4,8,11-Tetraazacyclotetradecane-5,7-dionato(2−)]platinum(*II*), 11CI

[106007-06-1]



M 421.3
First Pt complex of N_4 macrocycle with (2−) charge.
Synth. from diprotonated ligand + Tetrachloroplatinate(*II*)(2−), IC-017117 or from *cis* Diamminedichloroplatinum(*II*), IC-016643 + $S_2O_3^{2\ominus}$.
White needles (H_2O).

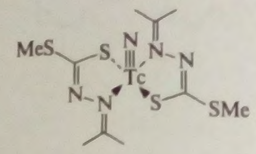
Kimura, E. *et al*, *J. Chem. Soc., Chem. Commun.*, 1986, 1020 (*synth, ir, uv*)

$C_{10}H_{18}N_5S_4Tc$ IC-007026

Bis(*S*-methyl-3-isopropylidenedithiocarbazato)nitridotechnetium(*V*)

Bis[*methyl*-(*1-methylethylidene*)*hydrazinecarbodithioato*-N^2,S^1]*nitridotechnetium, 12CI*

[115862-81-2]

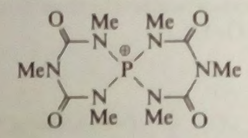


M 435.4
Synth. from $TcNCl_4^{\ominus}$ + ligand in $EtOH/CH_2Cl_2$ or from $TcNCl_2(PPh_3)_2$ + ligand in C_6H_6. Yellow solid ($EtOH/CH_2Cl_2$). Sol. CH_2Cl_2, $CHCl_3$, Me_2CO; insol. most other common solvs.

Marchi, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1988, 1743 (*synth, cryst struct, ir, pmr*)

$C_{10}H_{18}N_6O_4P^{\oplus}$ IC-007027

1,3,5,7,9,11-Hexamethyl-2,4,8,10-tetraoxo-1,3,5,7,9,11-hexaaza-6-phosphoniaspiro[5.5]undecane, 8CI



M 317.2 (ion)

Hexafluorophosphate: [33152-44-2].
White cryst. Mp 110-112°. $Subl._{0.5}$ 120°.

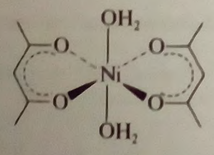
Dunmur, R.E. *et al*, *J. Chem. Soc. A*, 1971, 1289 (*synth, pmr, F-19 nmr, P-31 nmr*)

$C_{10}H_{18}NiO_6$ IC-007028

Diaquabis(2,4-pentanedionato-*O*,*O*′)nickel(*II*), 8CI

Nickel acetylacetonate dihydrate

[14024-81-8]



M 292.9
Octahedral sruct. Only known in *trans*-config. Synth. from Nickel(*II*) acetate, IC-004029 or Nickel(*III*) hydroxide oxide (Ni(OH)O), IC-019306 and pentanedione. Blue-green plates (Me_2CO/pet. ether). Vacuum sublimation gives Bis(2,4-pentanedionato-*O*,*O*′)nickel(*II*), IC-006926-9.

[35084-10-7, 36449-52-2]

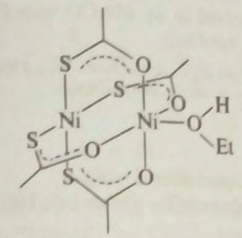
Montgomery, H. *et al*, *Acta Crystallogr.*, 1964, **17**, 1481 (*cryst struct*)
Hitchman, M.A. *et al*, *J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 846 (*uv*)
Battacharjee, M.N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 2561 (*synth*)

$C_{10}H_{18}Ni_2O_5S_4$ IC-007029

Tetrakis(μ-ethanethioato)ethanoldinickel, 9CI

(Ethyl alcohol)tetrakis(μ-thioacetato)dinickel, 8CI

[26896-74-2]



M 463.8
Believed to have dimeric struct. shown to account for phys. props., perhaps with Ni—S intermolecular interactions. Rare reports of Nickel(*II*) thioacetate probably refer to this compd. Synth. from basic Ni carbonate + thioacetic acid in EtOH. Dark red cryst. (EtOH). Sol. EtOH. Paramagnetic. $PhCOS^{\ominus}$ analogue known. Dec. at 150°.

Monomer: Bis(thioacetato)nickel(II), *8CI*
$C_4H_6NiO_2S_2$ M 208.9
Not thought to have any separate existence.

[20727-03-1, 41322-48-9]

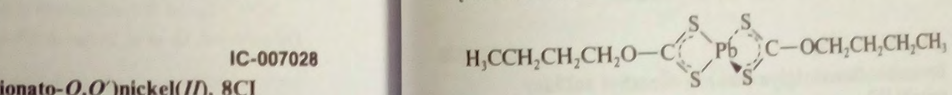
Melson, G.A. *et al*, *Inorg. Chem.*, 1970, **9**, 1123 (*synth, uv, magnetism*)

$C_{10}H_{18}O_2PbS_4$ IC-007030

Bis(*O*-butyl dithiocarbonato)lead

(O-Butyl carbonodithioato-S,S′)lead. Carbonodithioic acid, O-butyl ester lead(2+) salt, 9CI. Lead(II) *n-butylxanthate*

[16839-20-6]



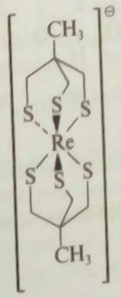
M 505.7
Formed in the flotation of sulfide minerals by xanthates.

Sasaki, Y., *Bunseki Kagaku*, 1982, **31**, E107; *CA*, **96**, 224110f (*formn const*)

$C_{10}H_{18}ReS_6^{\ominus}$ IC-007031

Bis[2-(mercaptomethyl)-2-methyl-1,3-propanedithiolato-*S*,*S*′]rhenate(*V*)(1−), 11CI

Bis(2-methyl-2-sulfidomethyl-1,3-propanedithiolato) rhenate(V)(*1*−)



M 516.8 (ion)
Trigonal prismatic anion, Re—S (av.) 233 pm.

Ph_4P salt: [84724-49-2].

Synth. from K_2ReCl_6 and 3 equivs. of H_3CCOCH_2SH in MeOH in presence of Et_3N followed by Ph_4PCl. Dark red cryst. (CH_2Cl_2/MeOH).

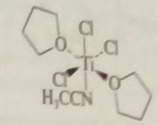
Blower, P.J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1986, 1339 (*synth, ir, pmr, cryst struct*)

$C_{10}H_{19}Cl_3NO_2Ti$ IC-007032

(Acetonitrile)trichlorobis(tetrahydrofuran)titanium(*III*)

Titanium(III) *chloride acetonitrile bis(tetrahydrofuran)*

[34384-13-9]



M 339.5
Distorted octahedral struct. The analogue with one THF is also known. Synth. by dissolving $TiCl_3$.3THF in THF and adding MeCN. Paramagnetic: μ_{eff} = 1.77μ_B, g = 1.909 (297K). μ_{eff} = 1.60μ_B, g = 1.909 (77K).

mer-form [76739-34-9]
Blue solid. Sol. THF, insol. hexane.

[82332-87-4]

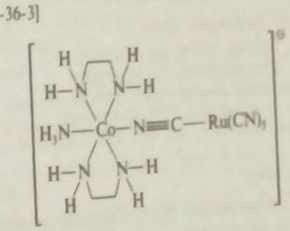
Hoff, G.R. *et al*, *Inorg. Chem.*, 1971, **10**, 2063 (*synth, ir, uv-vis, magnetism, esr*)
Zikmund, M. *et al*, *Chem. Zvesti*, 1982, **36**, 185; *CA*, **97**, 48348z (*magnetism, esr, mono-THF analogue*)
Piesch, G., *Chem. Zvesti*, 1984, **38**, 33; *CA*, **100**, 182499h (*electronic spectra*)

$C_{10}H_{19}CoN_{11}Ru^{\ominus}$ IC-007033

[Amminebis(1,2-ethanediamine-*N*,*N*′)cobaltate][μ-(cyano-*C*:*N*)][pentakis(cyano-C)ruthenate(1−), 11CI

Amminebis(ethylenediamine)cobalt(III)-*μ-cyano*(*pentacyano*) *ruthenate*(II)

[80481-36-3]



M 453.3 (ion)
Prepd. in soln. Not isol. as a solid.

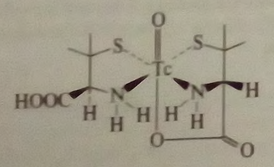
Bagger, S. *et al*, *Acta Chem. Scand., Ser. A*, 1981, **35**, 509 (*synth, uv, cmr, electrochem*)

$C_{10}H_{19}N_2O_5S_2Tc$ IC-007034

Bis(3-mercaptovalinato)oxotechnetium(*V*), 9CI

Bis(penicillaminato)technetium(V). *1-Oxo-2,3,6-(D-Oxobis(penicillaminato-S,N,O)-4,5-(D-penicillaminato-N,S) technetium*(V). *Bis(2-amino-3-mercapto-3-methylbutanoato-N,S)oxotechnetium*(V)

[80572-91-4]



D,D-penicillaminato-form

M 410.3

May also exist as $TcO(pen)_2^{2\ominus}$ and in binuclear form. Synth. from $[TcCl_6]^{2\ominus}$ or $[TcO_4]^{\ominus}$ + ligand. Has been used for renal imaging (kit TPEN). Yellow compd., may be reduced to a green Tc^{IV} species also obtainable by ligand exchange from $[TcBr_6]^{2\ominus}$.

Robinson, R.G. *et al*, *Int. J. Appl. Radiat. Isot.*, 1977, **28**, 919 (*synth, biodistribn*)
Johannsen, B. *et al*, *J. Nucl. Med.*, 1978, **19**, 816 (*synth, chromatog, electrochem, partition coeff, biodistribn*)
Yokoyama, A. *et al*, *J. Labelled Compd. Radiopharm.*, 1979, **16**, 80 (*synth, uv, chromatog, pharmacol*)
Davison, A. *et al*, *Acta Crystallogr., Sect. A*, 1981, **37**, C239 (*cryst struct*)
Franklin, K.J. *et al*, *Inorg. Chem.*, 1982, **21**, 1941 (*cryst struct*)

$C_{10}H_{20}AuO_4PS$ IC-007035

[Mercaptobutanedioato(1 –)]triethylphosphinegold, 9CI

$[Et_3PAuSCH(COOH)CH_2COOH]_n$

M 464.2

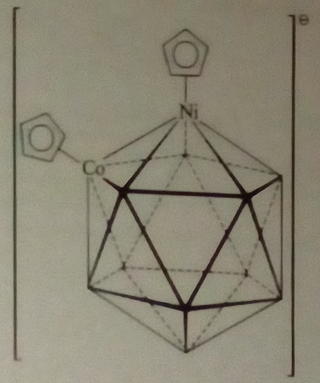
Polymeric. Antiarthritic drug.

U.S. Pat., 3 718 679, (1973); *CA*, **78**, 135672.
U.S. Pat., 3 718 680, (1973); *CA*, **78**, 135673.
Sadler, P.J., *Struct. Bonding (Berlin)*, 1976, **29**, 171 (*rev*)
Lorber, A. *et al*, *Gold Bull.*, 1979, **12**, 149 (*rev*)
Brown, D.H. *et al*, *Chem. Soc. Rev.*, 1980, **9**, 217 (*rev*)

$C_{10}H_{20}B_{10}CoNi^{\ominus}$ IC-007036

(η⁵-2,4-Cyclopentadien-1-yl)[(η⁵-2,4-cyclopentadien-1-yl) nickelate][μ-[η⁴:η⁴-decahydrodecaborato(4 –)]] cobaltate(1 –), 10CI

[68053-38-3]



M 366.0 (ion)

closo-. Synth. from *nido*-$[(\eta^5\text{-}C_5H_5Ni)B_{10}H_{12}]^{\ominus}$ + cobaltocene in 1,2-dimethoxyethane with Na/Hg.

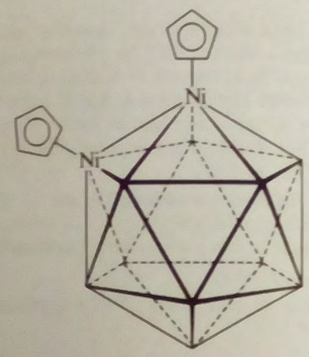
Ph_4As salt: Synth. from *nido*-$[(\eta^5\text{-}C_5H_5Ni)\text{-}B_{10}H_{12}]^{\ominus}$ + cobaltocene with Na/Hg in 1,2-dimethoxyethane. Residue dissolved in aq. Me_2CO with Ph_4AsCl added. Bright green needles.

Hawthorne, M.F. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3758 (*synth, pmr, B-11 nmr, ir, uv-vis, electrochem*)

$C_{10}H_{20}B_{10}Ni_2$ IC-007037

Bis(η⁵-2,4-cyclopentadien-1-yl)[μ-[decahydrodecaborato(2 –)]]dinickel, 10CI

[72104-70-2]



M 365.7

closo-. Proposed struct. shown. Various synth., e.g. from $[(C_5H_5)_3Ni_2]BF_4$ and $K_2B_{10}H_{10}$ in 1,2-dimethoxyethane. Golden brown solid.

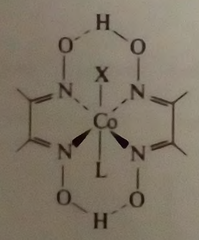
Hawthorne, M.F. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 3758 (*synth, B-11 nmr, pmr, ms, ir, uv-vis, electrochem*)

$C_{10}H_{20}BrCoN_4O_4S$ IC-007038

Bromobis(dimethylglyoximato)(dimethyl sulfide) cobalt(*III*)

Bromobis[2,3-butanedionedioximato(1 –)-N,N′] (thiobismethane)cobalt, 10CI

[79680-14-1]



L = SMe_2 , X = Br

M 431.1

Air stable brown cryst. Sol. CH_2Cl_2, $CHCl_3$, Me_2CO, THF.

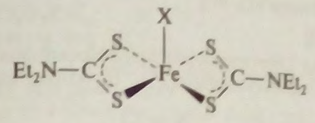
Inorg. Synth., 1980, **20**, 128 (*synth, ir, pmr*)

$C_{10}H_{20}BrFeN_2S_4$ IC-007039

Bromobis(*N,N*-diethyldithiocarbamato)iron(*III*)

Bromobis(diethylcarbamodithioato-S,S′)iron(III), *9CI*

[14879-23-3]



X = Br

M 432.2

Square pyramidal, Fe 59.5 pm above basal plane. Black cryst. ($CHCl_3$/toluene). Sol. $CHCl_3$, Me_2CO. Mp 230-235°. Exists in two cryst. mods., one form orders ferromagnetically at 1.347K. $S = \frac{1}{2}$ system; $\mu_{eff} = 4.07\mu_B$.

[54163-77-8]

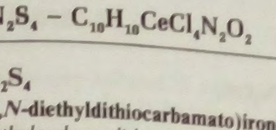
Martin, R.L. *et al*, *Inorg. Chem.*, 1967, **6**, 712 (*synth, ir, magnetism, uv-vis*)
Brackett, G.C. *et al*, *J. Chem. Phys.*, 1971, **54**, 4383 (*ir*)
Chapps, G.E. *et al*, *J. Chem. Phys.*, 1974, **60**, 990 (*esr, pmr, mössbauer, magnetism, cryst struct*)
Yoshikawa, M. *et al*, *Chem. Phys. Lett.*, 1981, **77**, 54 (*magnetism*)
Decurtins, S. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 1218 (*cryst struct, mössbauer*)

$C_{10}H_{20}Br_2MoN_2OS_4$ IC-007040

Dibromobis(diethyldithiocarbamato)oxomolybdenum(*VI*)

Dibromobis(diethylcarbamodithioato-S,S′) oxomolybdenum(VI), *9CI*

[53548-92-8]



X = Br

M 568.2

Pentagonal bipyramidal. Light yellow cryst. (CH_2Cl_2/Et_2O).

Dirand, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 278 (*cryst struct, synth*)
Lumpkin, O. *et al*, *Inorg. Chem.*, 1979, **18**, 982 (*O-17 nmr*)
Chen, G.J.J., *Inorg. Chim. Acta*, 1980, **41**, 49 (*props*)
Bradbury, J., *Inorg. Chem.*, 1986, **25**, 4408 (*props*)

$C_{10}H_{20}Br_3RuS_4$ IC-007041

(1,4,8,11-Tetrathiacyclotetradecane) tribromoruthenium(*III*)

As (1,4,8,11-Tetrathiacyclotetradecane) trichlororuthenium(*III*), IC-007051 with

X = Br

M 609.3

The ligand is only believed to be tridentate. Prepd. from (1,4,8,11-Tetrathiacyclotetradecane) trichlororuthenium(*III*), IC-007051 + LiBr in boiling Me_2CO. Brown-purple solid. $\mu_{eff} = 1.60\mu_B$.

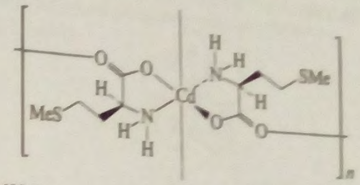
Ali, R. *et al*, *Inorg. Chim. Acta*, 1984, **84**, 65 (*synth, ir, uv, epr, magnetochem*)

$C_{10}H_{20}CdN_2O_4S_2$ IC-007042

Bis(L-methioninato-*N,O*)cadmium

Cadmium S-methionate

[51041-13-5]



M 408.8

6-Coord. Cd in polymeric solid state struct. Cryst. (H_2O).

[51041-14-6]

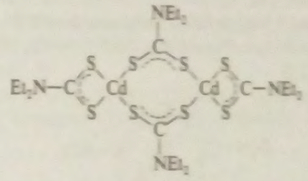
Flook, R.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 733 (*synth, cryst struct*)

$C_{10}H_{20}CdN_2S_4$ IC-007043

Bis(*N,N*-diethyldithiocarbamato)cadmium

Bis(diethylcarbamodithioato-S,S′)cadmium. Cadmium diethyldithiocarbamate

[14239-68-0]



dimer

M 408.9

Struct. is dimeric with one of the ligands forming a chelate ring and the other a bridge. Prepd. from Cd^{2+} + Et_2NCS_2Na.

▷ EU9850000.

Dimer:
$C_{20}H_{40}Cd_2N_4S_8$ M 817.9
White cryst. Mp 255°.

Shugam, E.A. *et al*, *Kristallografiya*, 1968, **13**, 253; *CA*, **69**, 39516x (*cryst struct*)
Nikolov, G.S. *et al*, *J. Inorg. Nucl. Chem.*, 1971, **33**, 1059 (*uv*)
Golding, R.M. *et al*, *Aust. J. Chem.*, 1972, **25**, 2567 (*ir, pmr*)
Bond, A.M. *et al*, *Aust. J. Chem.*, 1981, **34**, 1393 (*C-13 nmr*)
Riekkola, M.L. *et al*, *Acta Chem. Scand., Ser. A*, 1983, **37**, 691 (*ms*)
Geloso, C. *et al*, *Can. J. Chem.*, 1987, **65**, 928 (*synth*)
Frigerio, A. *et al*, *Inorg. Chim. Acta*, 1989, **164**, 149 (*synth, ir, raman*)
Sax, N.I. *et al*, *Dangerous Properties of Industrial Materials*, 7th Ed., Van Nostrand-Reinhold, 1989, **2**, 491.

$C_{10}H_{10}CeCl_4N_2O_2$ IC-007044

Tetrachlorobis(pyridine-1-oxide-*O*)cerium(*IV*)

Cerium(IV) *chloride bis(pyridine* N-*oxide)*

[114642-32-9]

$CeCl_4(C_5H_5NO)_2$

M 482.2

Yellow solid.

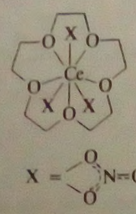
Li, W. *et al*, *Zhongguo Xitu Xuebao*, 1987, **5**, 65 (*synth, ir, pmr, pe*)

$C_{10}H_{20}CeN_3O_{14}$ IC-007045

(15-Crown-5)tris(nitrato)cerium(*III*)

Tris(nitrato-O,O')(1,4,7,10,13-pentaoxacyclopentadecane-$O^1,O^4,O^7,O^{10},O^{13}$)cerium(III), *10CI*

[67216-25-5]



M 546.3

11-Coordinate. Colourless cryst. Sol. MeCN. $\mu_{eff} = 2.36\mu_B$ (2.26K).

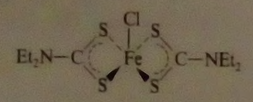
Bünzli, J.-C.G. *et al, Helv. Chim. Acta*, 1978, **61**, 1454 (*synth, ir*)
Lin Young-Hua, *et al, Huaxue Xuebao*, 1983, **41**, 97; *CA*, **98**, 207964 (*cryst struct*)
Liang, Y. *et al, Huaxue Xuebao*, 1983, **41**, 198; *CA*, **99**, 113138 (*ir, raman*)
Inorg. Synth., 1985, **23**, 151 (*synth, ir, magnetism*)

$C_{10}H_{20}ClFeN_2S_4$ IC-007046

Chlorobis(*N,N*-diethyldithiocarbamato)iron(*III*)

Chlorobis(diethylcarbamodithioato-S,S')*iron*(III), *9CI*

[14879-22-2]



M 387.8

Square pyramidal. Synth. from $(Et_2NCS_2)_3Fe$ + conc. HCl or by photolysis of $(Et_2NCS_2)_3Fe$ in $CHCl_3$ or PhCl. Catalyst for alkene hydrogenation or halogenation. Black cryst. Sol. Me_2CO, $CHCl_3$; insol. CCl_4, C_6H_6. Mp 250-255°. $\mu_{eff} = 4.00\mu_B$; ferromagnetic transition at 2.43K. $S = \frac{5}{2}$ system.

[36759-32-7]

Martin, R.L. *et al, Inorg. Chem.*, 1967, **6**, 712 (*synth, magnetism, ir*)
Wickman, H.H. *et al, Phys. Rev.*, 1967, **155**, 563 (*magnetism, mössbauer*)
Wickmann, H.H. *et al, Inorg. Chem.*, 1968, **7**, 63.
Hoskins, B.F. *et al, J. Chem. Soc. A*, 1970, 1668 (*cryst struct*)
de Vries, J.L.K.F. *et al, Inorg. Chem.*, 1971, **10**, 81.
Brackett, G.C. *et al, J. Chem. Phys.*, 1971, **54**, 4383 (*ir*)
Wickman, H.H., *J. Chem. Phys.*, 1972, **56**, 976 (*magnetism, mössbauer*)
Chapps, G.E. *et al, J. Chem. Phys.*, 1974, **60**, 990 (*magnetism, esr, mössbauer*)
Dhingra, M.M. *et al, J. Magn. Reson.*, 1975, **20**, 133 (*pmr*)
Miessler, G.L. *et al, Inorg. Chem.*, 1976, **15**, 1982 (*synth, ir*)
De Fotis, G.C. *et al, J. Am. Chem. Soc.*, 1977, **99**, 8314 (*magnetism*)
Giren, K.W. *et al, J. Inorg. Nucl. Chem.*, 1977, **39**, 1309 (*ms*)
Bhatia, S.N. *et al, Proc. Nucl. Phys. Solid State Phys. Symp., C*, 1977, **20**, 424 (*magnetism*)
Coucouvanis, D., *Prog. Inorg. Chem.*, 1979, **26**, 301 (*rev, bibl*)
Katsaulos, G.A., *Can. J. Chem.*, 1985, **63**, 3249 (*complexes*)
Tsipis, C.A. *et al, J. Chem. Soc., Chem. Commun.*, 1985, 1404 (*use*)

$C_{10}H_{20}Cl_2MoN_2OS_4$ IC-007047

Dichlorobis(*N,N*-diethyldithiocarbamato)oxomolybdenum(*VI*)

Dichlorobis(diethylcarbamodithioato-S,S')*oxomolybdenum*(VI), *9CI*

[57146-54-0]

As Dibromobis(diethyldithiocarbamato)oxomolybdenum(*VI*), IC-007040 with

X = Cl

M 479.3

Pentagonal bipyramidal. Light yellow cryst. (CH_2Cl_2/Et_2O).

Dirand, J. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 278 (*cryst struct, synth*)
Chen, G.J.J., *Inorg. Chim. Acta*, 1980, **41**, 49 (*props*)
Bradbury, J., *Inorg. Chem.*, 1986, **25**, 4408 (*props*)

$C_{10}H_{20}Cl_2N_2ReS_4$ IC-007048

Dichlorobis(*N,N*-diethyldithiocarbamato)rhenium(*IV*)

Dichlorobis(diethylcarbamodithioato-S,S')*rhenium*(IV), *10CI, 9CI*

[41904-51-2]

$ReCl_2(S_2CNEt_2)_2$

M 553.6

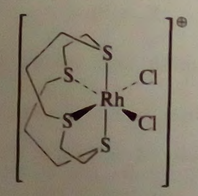
Synth. from Tetrachlorobis(triphenylphosphine)rhenium(*IV*), IC-013232 and $(Et_2NCS_2)_2$ in C_6H_6. Red cryst.

[52646-86-3]

Rowbottom, J.F. *et al, J. Chem. Soc., Dalton Trans.*, 1974, 684 (*synth, ir, props*)

$C_{10}H_{20}Cl_2RhS_4^{\oplus}$ IC-007049

Dichloro(1,4,8,11-tetrathiacyclotetradecane)rhodium(*III*) (1+), 9CI



M 442.3 (ion)

cis-Config. only.

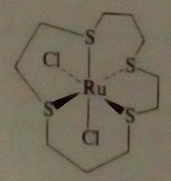
Chloride: [52393-01-8].

Bright yellow microcryst. Sol. $MeNO_2$.

Travis, K. *et al, Inorg. Chem.*, 1974, **13**, 2591 (*synth, ir, uv*)

$C_{10}H_{20}Cl_2RuS_4$ IC-007050

Dichloro(1,4,8,11-tetrathiacyclotetradecane)ruthenium(*II*)



cis-form

M 440.5

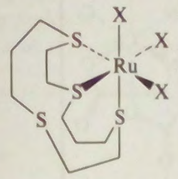
Originally incorrectly assigned as *trans*-isomer. Ru—Cl 247.1, Ru—$S_{(transtoCl}$ 226.2; Ru—$S_{transtoS}$ 233.3 pm. Prepd. by boiling $K_2[RuCl_5(OH_2)]$ with ligand in $H_3COC_2H_4OH$ for 2 d.

Di-hydrate:
$C_{10}H_{24}Cl_2O_2RuS_4$ M 476.5
Orange cryst. (aq. HCl).

Poon, C.-K. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 756; 1981, 494; 1982, 1457 (*synth, uv, ir*)
Lai, T.-F. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 1465 (*cryst struct, ir*)

$C_{10}H_{20}Cl_3RuS_4$ IC-007051

(1,4,8,11-Tetrathiacyclotetradecane)trichlororuthenium(*III*)



fac-form

X = Cl

M 475.9

The ligand is only believed to be tridentate. Prepd. by treating $RuCl_3.xH_2O$ with ligand in boiling EtOH. Brown solid. $\mu_{eff} = 1.71\mu_B$.

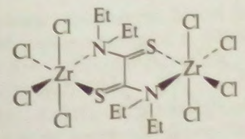
Ali, R. *et al, Inorg. Chim. Acta*, 1984, **84**, 65 (*synth, ir, uv, epr, magnetism*)

$C_{10}H_{20}Cl_8N_2S_2Zr_2$ IC-007052

Octachloro[μ-(tetraethylethanedithioamide-$N^1,S^2:N^2,S^1$)]dizirconium(*IV*), 11Cl

Octachloro[μ-(tetraethyldithiooxamide-$N^1,S^2:N^2,S^1$)]*dizirconium*(IV)

[96321-23-2]



M 698.4

Synth. from $ZrCl_4$ and the ligand in CH_2Cl_2. White moisture-sensitive solid which is a weak electrolyte in MeCN.

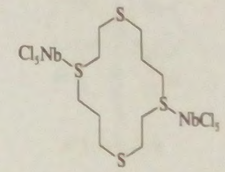
Martinez, M. *et al, Acta Cient. Compostelana*, 1983, **20**, 181; *CA*, **102**, 196725g (*synth, ir, uv*)

$C_{10}H_{20}Cl_{10}Nb_2S_4$ IC-007053

Decachloro[μ-(1,4,8,11-tetrathiacyclotetradecane-$S^1:S^4$)]diniobium(*V*), 10Cl

(μ-1,4,8,11-Tetrathiacyclotetradecane)bis[pentachloroniobium(V)]. *Niobium*(V) *chloride hemi(1,4,8,11-tetrathiacyclotetradecane) complex*

[55543-64-1]



M 808.8

Octahedral at Nb. Synth. by mixing C_6H_6 solns. of $NbCl_5$ and the ligand. Wine-red solid.

De Simone, R.E. *et al, J. Coord. Chem.*, 1976, **5**, 181 (*cryst struct*)
De Simone, R.E. *et al, J. Inorg. Nucl. Chem.*, 1976, **38**, 1623 (*synth, ir, pmr*)

$C_{10}H_{20}CrFN_8Ni$ IC-007054

[μ-(Cyano-*C*:*N*)]fluorobis(1,2-propanediamine-*N,N'*)[tris(cyano-*C*)nickel(*II*)]chromium(*III*), 11Cl

[*Bis(1,2-diaminopropane)fluorochromium*(III)]-μ-*cyano(tricyano)nickel*(II)

[86305-50-2]

As Bromo[μ-(cyano-*C*:*N*)]bis(1,2-ethanediamine-*N,N'*)[tris(cyano-*C*)nickel(*II*)]chromium(*III*), IC-006060 with

R = CH_3, X = F

M 382.0

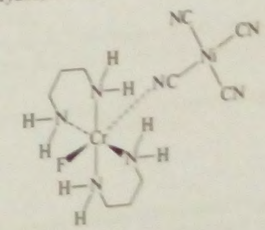
Binuclear complex with bridging CN. Suggested to have *cis*-configuration at Cr, but not confirmed. Obt. on heating $[CrF[C_3H_6(NH)_2]_2(H_2O)]^{2\oplus}(ClO_4)_2$ with NH_4 salt of Tetrakis(cyano-*C*)nickelate(2−), IC-004541.

Ribas, J. *et al, Transition Met. Chem.*, 1983, **8**, 87 (*synth, ir*)

$C_{10}H_{20}CrFN_8Ni$ IC-007055

[μ-(Cyano-*C*:*N*)]fluorobis(1,3-propanediamine-*N,N'*)[tris(cyano-*C*)nickel(*II*)]chromium(*III*)

[*Bis(1,3-diaminopropane)fluorochromium*(III)]-μ-*cyano(tricyano)nickel*(II)



M 382.0

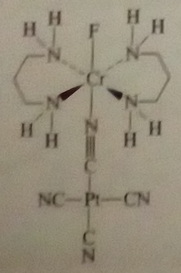
Suggested to have *trans*-config. but 1,2-diamine analogues believed to have *cis*-geometry, e.g. [μ-(Cyano-*C*:*N*)]fluorobis(1,2-propanediamine-*N,N'*)[tris(cyano-*C*)nickel(*II*)]chromium(*III*), 11Cl, IC-007054. Prepd. by heating Tetrakis(cyano-*C*)nickelate(2−), IC-004541 salt of $[Cr[C_3H_6(NH_2)_2]_2H_2O]^{3\oplus}$

Ribas, J. *et al, J. Inorg. Nucl. Chem.*, 1981, **43**, 3113 (*synth, ir, uv*)

$C_{10}H_{20}CrFN_3Pt$ IC-007056

(μ-Cyano-*C*:*N*)fluorobis(1,3-propanediamine-*N*,*N*′)tris(cyano-*C*)platinum]chromium, 1ICI

[Fluorobis(1,3-diaminopropane)chromium(III)]-μ-cyano[tricyanoplatinum(II)]



M 518.3

Yellow (?) solid. Insol. Note change of config. around Cr compared with corresp. chloride complex. Chloro(μ-cyano-*C*:*N*)bis(1,2-ethanediamine-*N*,*N*′)(tris(cyano-*C*) platinum)chromium, IC-006071.

Ribas, J. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 3113 (*synth, ir, uv*)

$C_{10}H_{20}CrN_2S_4$ IC-007057

Bis(*N*,*N*-diethyldithiocarbamato)chromium(*II*)

Bis(diethylcarbamodithioato-S,S′)chromium(II), 1ICI. Chromium(II) diethyldithiocarbamate

[15699-68-0]

$Cr(S_2CNEt_2)_2$

M 348.5

Possibly *S*-bridged dimer with approx. square pyramidal Cr(*II*). Yellow solid. μ_{eff} = 3.98 (300K), 2.21μ_B (90K). Antiferromagnetic.

▷ Pyrophoric.

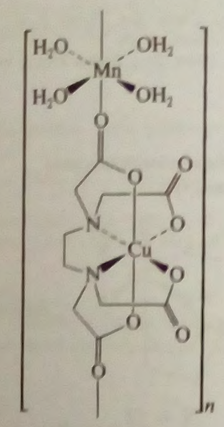
Fackler, J.P. *et al*, *Inorg. Nucl. Chem. Lett.*, 1966, **2**, 251 (*synth*)
Larkworthy, L.F. *et al*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 139 (*synth*)
Lancashire, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1982, 845.
Tanaka, M. *et al*, *Polyhedron*, 1986, **5**, 703.

$C_{10}H_{20}CuMnN_2O_{12}$ IC-007058

***catena*-Tetraaquamanganese(*II*)[μ-ethylenediaminetetraacetato]copper(*II*)**

Tetraaqua[[N,N′-1,2-ethanediylbis[N-(carboxymethyl) glycinato]](4 –)](copper)manganese, 10CI

[61628-25-9]



M 478.7

Synth. from $Mn(NO_3)_2$, $Cu(NO_3)_2$, H_4edta in H_2O. Cryst. + $2H_2O$.

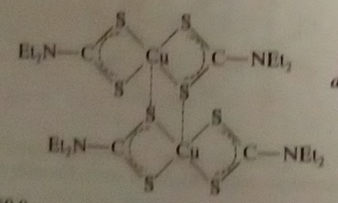
Solans, X. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 435 (*cryst struct*)
Eschriva, E. *et al*, *Transition Met. Chem.*, 1984, **9**, 184 (*synth, thermal props*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1987, **D5**, 42 (*rev, bibl*)

$C_{10}H_{20}CuN_2S_4$ IC-007059

Bis(*N*,*N*-diethyldithiocarbamato)copper(*II*)

Bis(diethylcarbamodithioato-S,S′)copper(II). Copper(II) diethyldithiocarbamate

[13681-87-3]



dimer

M 360.0

Weakly dimeric with distorted tetragonal-pyramidal coordination at Cu and negligible spin interaction.

▷ EZ5250000.

Dimer

$C_{20}H_{40}CuN_4S_8$ M 656.6

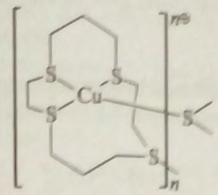
Air-stable deep green prismatic cryst.

Bonamico, M. *et al*, *Acta Crystallogr.*, 1965, **19**, 886 (*cryst struct*)
Lesz, K. *et al*, *Chem. Anal. (Warsaw)*, 1966, **11**, 523; *CA*, **65**, 14814 (*synth*)
Anufrienko, V.F. *et al*, *Teor. Eksp. Khim.*, 1967, **3**, 370; *CA*, **68**, 73940v (*esr*)
Hara, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1969, **42**, 576 (*magnetism*)
Di Ascenzo, G. *et al*, *J. Therm. Anal.*, 1969, **1**, 423 (*thermal props*)
Pilipenko, A.T. *et al*, *Zh. Neorg. Khim.*, 1969, **14**, 462 (*ir*)

$C_{10}H_{20}CuS_4^{\oplus}$ IC-007060

(1,4,8,11-Tetrathiacyclotetradecane)copper(*I*)(1+)

[93645-99-9]



M 332.0 (ion)

Stepwise chain polymer with tetrahedral coord. around Cu. Synthesised electrochemically.

Perchlorate: Cryst.

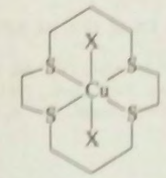
▷ Potentially explosive.

Dockal, E.R. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 4530 (*synth, cryst struct*)
Diaddario, L.L. *et al*, *Inorg. Chem.*, 1985, **24**, 356 (*synth, cryst struct*)

$C_{10}H_{20}CuS_4^{2\oplus}$ IC-007061

(1,4,8,11-Tetrathiacyclotetradecane-S^1,S^4,S^8,S^{11})copper(*II*)(2+), 9CI

[57673-86-6]



X = $OClO_3$

diperchlorate

M 332.0 (ion)

Cu in square planar environment. Model for blue copper proteins. The intense absorption at 600 nm is believed to involve a S→ Cu(*II*) charge transfer.

Diperchlorate: [58384-13-7].
Blue cryst. (aq. EtOH). Sol. MeOH; insol. H_2O. Perchlorate anions weakly coordinated to Cu.

▷ Potentially explosive.

Bis-tetrafluoroborate: [71120-59-7].
[57673-86-6, 63412-75-9, 93645-99-9]

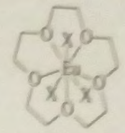
Jones, T.E. *et al*, *J. Am. Chem. Soc.*, 1975, **97**, 7163, 7485 (*uv, electrochem, esr*)
Glick, M.D. *et al*, *Inorg. Chem.*, 1976, **15**, 1190 (*cryst struct*)
Sakaguchi, U. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 600 (*esr, electrochem*)
Yamabe, T. *et al*, *Inorg. Chem.*, 1982, **21**, 2040 (*theory*)
Rorabacher, D.B. *et al*, *Copper Coord. Chem., Biochem. Inorg. Perspect., 1983*, (Karlin, K.D., *et al* Eds.), Adenine Press, Guilderland, N.Y., 1983, 169 (*electrochem*)
Brubaker, G.R. *et al*, *Inorg. Chem.*, 1984, **23**, 1591 (*stability constants*)
Scott, R.A. *et al*, *Biochemistry*, 1986, **25**, 5546 (*exafs*)

$C_{10}H_{20}EuN_3O_{14}$ IC-007062

(15-Crown-5)tris(nitrato)europium(*III*)

Tris(nitrato-O,O′)(1,4,7,10,13-pentaoxacyclopentadecane-O^1,O^4,O^7,O^{10},O^{13})europium. Europium(III) nitrate 15-crown-5

[67216-29-9]



X = NO_3

M 558.2

11-Coordinate with bidentate nitrate. Yellow cryst. Sol. MeCN. Paramagnetic; μ_{eff} = 3.31μ_B. Dec. > 170°.

Blinzli, J.-C.G. *et al*, *Inorg. Chem.*, 1982, **21**, 808 (*synth, cryst struct, luminesc*)
Liang, Y. *et al*, *Huaxue Xuebao*, 1983, **41**, 198; *CA*, **99**, 113138 (*ir, raman*)
Inorg. Synth., 1985, **23**, 149 (*synth, ir, raman*)

$C_{10}H_{20}FeIN_2S_4$ IC-007063

Bis(*N*,*N*-diethyldithiocarbamato)iodoiron(*III*)

Bis(diethylcarbamodithioato-S,S′)iodoiron(III), 8ICI

[14879-24-4]

As Bromobis(*N*,*N*-diethyldithiocarbamato)iron(*III*), IC-007039 with

X = I

M 479.2

Contains rare Fe(*III*)—I bond. Square pyramidal Fe 59 pm above basal plane. Black cryst. Sol. $CHCl_3$, CH_2Cl_2, Me_2CO. Mp 220-225°. $S = \frac{1}{2}$ system; μ_{eff} = 3.88μ_B (293K).

[38246-70-7]

Martin, R.L. *et al*, *Inorg. Chem.*, 1967, **6**, 712 (*synth, ir, uv-vis, magnetism*)
Healy, P.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 1389 (*cryst struct*)
Chapps, G.E. *et al*, *J. Chem. Phys.*, 1974, **60**, 990 (*esr, pmr, mössbauer, magnetism*)
Mve Ondo, B. *et al*, *Comp. Rend. Hebd. Seances Acad. Sci. Sect. C*, 1985, **301**, 225 (*synth*)

$C_{10}H_{20}FeI_3N_2S_4$ IC-007064

Bis(*N*,*N*-diethyldithiocarbamato)(triiodo)iron(*III*)

Bis(diethylcarbamodithioato-S,S′)(triiodo)iron(III)

[62171-16-8]

As Bromobis(*N*,*N*-diethyldithiocarbamato)iron(*III*), IC-007039 with

X = I_2

M 733.1

Believed to contain I_2 group with terminal I bound to Fe. 5-coord. Fe with $S = \frac{1}{2}$ ground state. Black cryst. (CH_2Cl_2/cyclohexane). Sol. CH_2Cl_2. Mössbauer studies at 4.2K indicate three non equivalent iodine atoms.

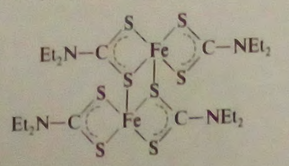
Pasek, E.A. *et al*, *Inorg. Chim. Acta*, 1977, **21**, 23 (*synth, mössbauer, uv-vis*)
Petrilis, D. *et al*, *Inorg. Chem.*, 1982, **21**, 786 (*mössbauer*)

$C_{10}H_{20}FeN_2S_4$ IC-007065

Bis(*N,N*-diethyldithiocarbamato)iron(*II*)

Bis(diethylcarbamodithioato-S,S′)iron(II), *11CI*

[15656-03-8]



dimer

M 352.3

Dimeric in solid state. Catalyst, biocide.

Dimer:

$C_{20}H_{40}Fe_2N_4S_8$ M 704.7

Synth. from $FeSO_4$ + 2 NaS_2CNEt_2. Air-sensitive dark-red cryst. Mp ~230°.

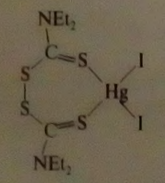
Pignolet, L.H. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 360 (*synth*)
de Vries, J.L.K. *et al*, *Inorg. Chem.*, 1973, **12**, 2730 (*mössbauer, synth, magnetism*)
Ileperuma, O.A. *et al*, *Inorg. Chem.*, 1975, **14**, 3042 (*cryst struct*)
Bond, A.M. *et al*, *Coord. Chem. Rev.*, 1984, **54**, 23 (*rev, bibl*)

$C_{10}H_{20}HgI_2N_2S_4$ IC-007066

Bis[(diethylthiocarbamoyl)disulfide]diiodomercury

[*Bis*[(*diethylamino*)*thioxomethyl*]*disulfide*]*diiodomercury*. *Diiodo*(*tetraethylthiuram disulfide*)*mercury*. *Bis*[(*diethylthiocarbamoyl*)*disulfide*]*mercury diiodide*

[27821-89-2]



M 750.9

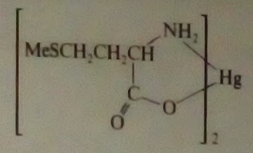
Monomeric in solid state. Yellow plates (pet. ether). Sol. $CHCl_3$. Mp 132.5-136°.

Brinckhoff, H.C. *et al*, *Recl. Trav. Chim. Pays-Bas* (*J. R. Neth. Chem. Soc.*), 1970, **89**, 11; 1971, **90**, 252 (*ir, pmr, synth, ir*)
Chieh, C., *Can. J. Chem.*, 1977, **55**, 1115 (*synth, cryst struct*)
Van Gaal, H.L.M. *et al*, *Inorg. Chem.*, 1979, **18**, 351 (*cmr, ir*)

$C_{10}H_{20}HgN_2O_4S_2$ IC-007067

Bis(methionato)mercury

Mercury methionate



M 497.0

In the solid state, Hg is bonded by amino N and carboxyl O whereas in soln., Hg bonding is localised to the S of methionine.

DL-form [31210-58-9]

Prepd. by reaction of $Hg(OAc)_2$ with DL-methionine. Cryst.

▷ OV7369400.

[15283-03-1, 51311-30-9, 52611-12-8]

Natusch, D.F.S. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 596 (*nmr, bonding*)
Birgersson, B. *et al*, *Acta Chem. Scand.*, 1973, **27**, 3953 (*synth, pmr, cmr*)
Sze, Y.K. *et al*, *Inorg. Chem.*, 1975, **14**, 1969 (*ir, raman, bonding*)

$C_{10}H_{20}HgN_2S_4$ IC-007068

Bis(*N,N*-diethyldithiocarbamato)mercury

Bis(diethylcarbamodithioato-S,S′)mercury, 9CI

[14239-51-1]

$Hg[S_2CNEt_2]_2$

M 497.1

Two forms: α-dimeric: 5-coord. (similar to Zn and Cd analogues), β-form weakly associated monomers (via Hg...S) forming a helical quasipolymeric array. Yellow cryst. (Me_2CO). Mp 127-130° (136°).

▷ OV7360000.

Dimer: [50982-16-6]. *Bis*[*μ*-(*diethylcarbamodithioato-S:S,S′*)] *bis*(*diethylcarbamodithioato-S,S′*)*dimercury*

$C_{20}H_{40}Hg_2N_4S_8$ M 994.2

[41078-90-4, 50797-96-1]

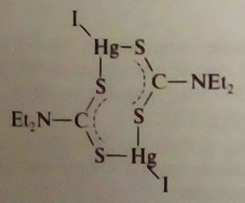
Iwasaki, H. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 2115 (*synth, cryst struct, α- and β-forms*)
Healy, P.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 284 (*synth, cryst struct, β-form*)
Frost, D.C. *et al*, *J. Electron Spectrosc. Relat. Phenom.*, 1975, **7**, 297 (*pe*)
Chieh, C. *et al*, *Can. J. Chem.*, 1976, **54**, 3077 (*raman, ir, α- and β-forms*)
Bond, A.M. *et al*, *Aust. J. Chem.*, 1981, **34**, 1393 (*Hg-199 nmr*)
Kellner, R. *et al*, *J. Inorg. Nucl. Chem.*, 1981, **43**, 1183 (*ir*)
Riekkola, M.L., *Acta Chem. Scand., Ser. A*, 1983, **37**, 691 (*ms*)

$C_{10}H_{20}Hg_2I_2N_2S_4$ IC-007069

Bis(*N,N*-diethyldithiocarbamato)diiododimercury(*II*)

Bis[*μ*-(*diethylcarbamodithioato-S:S′*)]*diiododimercury, 10CI*

[64012-17-5]



M 951.5

Yellow platelets. Mp 136°.

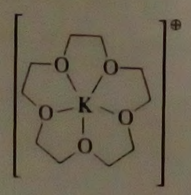
Chieh, C., *Can. J. Chem.*, 1977, **55**, 65 (*synth, cryst struct, raman*)
Yusuff, K. *et al*, *Synth. React. Inorg. Metal-Org. Chem.*, 1989, **19**, 15 (*synth*)

$C_{10}H_{20}KO_5^{\oplus}$ IC-007070

(15-Crown-5)potassium(1+)

(*1,4,7,10,13-Pentaoxacyclopentadecane*)*potassium*(*1+*), *10CI*

[61060-13-7]



M 259.3 (ion)

In the salt with $Cu_4I_6^{2\ominus}$, the K ion is located above the

plane of the five heteroatoms of the cyclic ether and has ionic contacts to three I atoms. Prepd. by reaction of required K salt with 15-crown-5 in MeOH. log K_s 0.74 (H_2O), ΔH −17.3 kJ mol^{-1} (complex formn. H_2O), log K_s 3.77 (MeOH), ΔH −32.2 kJ mol^{-1} (complex formation MeOH).

Di-μ-iodotetraiodobicuprate(*2−*) *salt* (*2:1*): [98931-67-0].

$C_{20}H_{40}Cu_2I_6K_2O_{10}$ M 1407.2

Prepd. by addition of an Me_2CO soln. of ligand to CuI in aq. KI. Cryst.

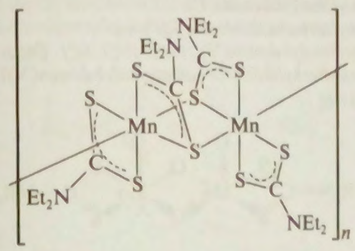
Izatt, R.M. *et al*, *J. Am. Chem. Soc.*, 1976, **98**, 7620 (*thermodyn*)
Lamb, J.D. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 475 (*thermodyn*)
Miyazaki, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 2005 (*use*)
Rath, N.P. *et al*, *J. Chem. Soc., Chem. Commun.*, 1985, 665 (*cryst struct*, $Cu_4I_6^{2\ominus}$ *salt*)
Eliasson, B. *et al*, *J. Phys. Chem.*, 1985, **89**, 258 (*cmr, O-17, K-39 nmr*)
Takeuchi, H. *et al*, *J. Mol. Struct.*, 1986, **146**, 197 (*raman*)
Ozkan, E. *et al*, *Spectrosc. Lett.*, 1986, **19**, 693 (*cmr, thermodyn*)

$C_{10}H_{20}MnN_2S_4$ IC-007071

Bis(*N,N*-diethyldithiocarbamato)manganese(*II*)

Bis(diethylcarbamodithioato-S,S′)manganese(II), *11CI*

[57683-09-7]



M 351.4

Possesses polymeric chain struct. with octahedral Mn. Synth. from $MnCl_2.4H_2O$ and $Na[S_2CNEt_2]$ in H_2O in the absence of oxygen. Yellow cryst. (EtOH), readily oxidised in air. Sol. Py; sl. sol. MeOH, EtOH, Me_2CO, CH_2Cl_2. Possesses temp. dependent magnetic moment and exhibits antiferromagnetic interactions.Other N-substituted derivs. known which are less air-sensitive. Forms bisadducts with N- heterocyclic ligands.

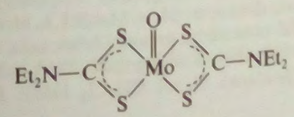
[15685-17-3]

Hendrickson, A.R. *et al*, *Inorg. Chem.*, 1974, **13**, 1933 (*electrochem*)
Hill, D.M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1726 (*magnetism*)
Ciampolini, M. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 2051 (*synth, cryst struct, magnetism*)
Coucouvanis, D., *Prog. Inorg. Chem.*, 1979, **26**, 301 (*rev, bibl*)
Jezierski, A., *J. Mol. Struct.*, 1984, **115**, 11 (*esr*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 139 (*rev, bibl*)

$C_{10}H_{20}MoN_2OS_4$ IC-007072

Bis(*N,N*-diethyldithiocarbamato)oxomolybdenum(*IV*)

[25395-92-0]



M 408.4

Synth. by abstraction of oxygen from $MoO_2(S_2CNEt_2)_2$ in CH_2Cl_2 with PPh_2Et. Starting material. Pink solid.

[63950-40-3]

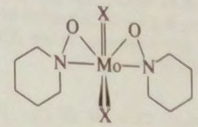
Chen, G.J.-J. *et al*, *Inorg. Chem.*, 1976, **15**, 2612 (*synth*)
Young, C.G. *et al*, *Inorg. Chem.*, 1985, **24**, 4416 (*Mo-95 nmr*)
Huang Liangren, *Jiegou Huaxue*, 1986, **5**, 124 (*cryst struct*)
Compr. Coord. Chem., 1987, **3**, 1336, 1339, 1391 (*rev*)

$C_{10}H_{20}MoN_2O_2S_2$ IC-007073

Bis(1-hydroxypiperidinato-*N*′,*O*′)dithioxomolybdenum(*VI*), 11CI

Bis(*piperidine*-N-*oxide*)*disulfidomolybdenum*(VI)

[84146-55-4]



X = S

M 360.3

cis-form

Mo=S 214.5 pm. Dark red cryst. (toluene). Diamagnetic. Resembles Bis(1-hydroxypiperidinato-N^1,O^1)dioxomolybdenum(*VI*), IC-007077.

[93493-29-9]

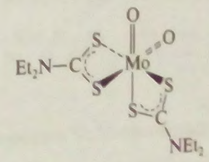
Wieghardt, K. *et al*, *Z. Anorg. Allg. Chem.*, 1982, **492**, 164 (*cryst struct, pmr, uv*)
Minelli, M. *et al*, *Inorg. Chem.*, 1983, **22**, 3952 (*Mo-95 nmr*)
Bristow, S. *et al*, *Inorg. Chim. Acta*, 1983, **76**, L261 (*reactions*)
Bristow, S. *et al*, *J. Chem. Soc., Dalton Trans.*, 1984, 1617 (*electrochem*)

$C_{10}H_{20}MoN_2O_2S_4$ IC-007074

Bis(*N,N*-diethyldithiocarbamato)dioxomolybdenum(*VI*)

Bis(diethylcarbamodithioato-S,S′)dioxomolybdenum(VI), *11CI, 10CI, 9CI*

[18078-69-8]



M 424.4

Synth. from $[MoO_4]^{2\ominus}$ + $Na[S_2CNEt_2]$. Catalyses oxidation by air of PPh_3 and PhCH(OH)COPh. Yellow cryst. (C_6H_6/pet. ether) or orange cryst. (hot toluene). Sl. sol. CH_2Cl_2, $CHCl_3$, Me_2CO, warm C_6H_6. Mp 133-133.5°. Ir $\nu_{Mo=O}$ 910, 877 cm^{-1} (KBr).

[19680-83-2]

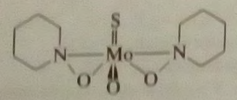
Moore, F.W. *et al*, *Inorg. Chem.*, 1967, **6**, 998 (*synth, ir, vis*)
Berg, J.M. *et al*, *Inorg. Chem.*, 1980, **19**, 2180 (*cryst struct*)
Christensen, K.A. *et al*, *Inorg. Chim. Acta*, 1981, **56**, L27 (*Mo-95 nmr*)
Cerny, R.L. *et al*, *Anal. Chem.*, 1983, **55**, 1954 (*ms*)
Chen, G.J.J. *et al*, *Inorg. Chem.*, 1985, **24**, 2327 (*synth, ir*)
Ueyama, N. *et al*, *J. Chem. Soc., Dalton Trans.*, 1985, 635 (*use*)

$C_{10}H_{20}MoN_2O_3S$ IC-007075

Bis(1-hydroxypiperidinato-N^1,O^1)oxothioxomolybdenum(*VI*), 11CI, 10CI

Oxobis(piperidine-N-*oxide*-N,O)*thiomolybdenum*(VI)

[84133-89-1]



M 344.2

First example of an $MoOS^{2\oplus}$ moiety, possible model for the Mo centre in the oxidised active form of xanthine oxidase and dehydrogenase. Yellow ($CHCl_3$) or orange-red cryst. (MeOH).

[93512-01-7]

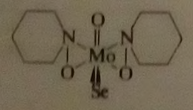
Hofer, E. *et al, Angew. Chem., Int. Ed. Engl.*, 1981, **20**, 282 (*synth*)
Wieghardt, K. *et al, Z. Anorg. Allg. Chem.*, 1982, **492**, 164 (*synth*)
Minelli, M. *et al, Inorg. Chem.*, 1983, **22**, 3952 (*Mo-95 nmr*)
Bristow, S. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 2495; 1984, 1617 (*cryst struct, synth, ir, pmr, cmr, Mo-95 nmr, raman, ms, electrochem*)

$C_{10}H_{20}MoN_2O_3Se$ IC-007076

Bis(1-hydroxypiperidinato-N^1,O^1)oxoselenoxomolybdenum(*VI*), 11CI

Oxobis(piperidine-N-*oxido*-O,N)*selenomolybdenum*(VI)

[84133-91-5]



M 391.1

Struct. closely related to S analogue. Mo—Se 229.9, Mo=O 171.9, Mo—O 196.1, 195.7 pm. Dark-red prisms (CH_2Cl_2/2-propanol). Indefinitely stable under N_2 at ambient temp.

Wieghardt, K. *et al, Z. Anorg. Allg. Chem.*, 1982, **492**, 164 (*synth, uv-vis, pmr*)
Minelli, M. *et al, Inorg. Chem.*, 1983, **22**, 3952 (*Mo-95 nmr*)
Traill, P.R. *et al, Aust. J. Chem.*, 1986, **39**, 1287 (*cryst struct*)

$C_{10}H_{20}MoN_2O_4$ IC-007077

Bis(1-hydroxypiperidinato-N^1,O^1)dioxomolybdenum(*VI*), 11CI

Dioxobis(piperidine-N-*oxide)molybdenum*(VI)

[84120-41-2]

As Bis(1-hydroxypiperidinato-N^1,O^1) dithioxomolybdenum(*VI*), IC-007073 with

X = O

M 328.2

Skew trapezoid bipyramid with sideways bonded ligand.

cis-form

Colourless cryst. (EtOH). Sol. CH_2Cl_2, $CHCl_3$, toluene. Diamagnetic.

[93493-30-2]

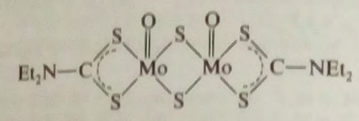
Wieghardt, K. *et al, Z. Anorg. Allg. Chem.*, 1982, **492**, 164 (*cryst struct, pmr, uv, ir*)
Minelli, M. *et al, Inorg. Chem.*, 1983, **22**, 3952 (*Mo-95 nmr*)
Bristow, S. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1617 (*electrochem*)
Bristow, S. *et al, Inorg. Chem.*, 1985, **24**, 4070 (*reactions*)
Bristow, S. *et al, Polyhedron*, 1986, **5**, 319 (*reactions*)

$C_{10}H_{20}Mo_2N_2O_2S_6$ IC-007078

Bis(diethylcarbamodithioato-*S,S'*)dioxodi-μ-thioxodimolybdenum(*V*), 11CI, 10CI, 9CI

Bis(μ_2-*sulfido*)*bis*[*oxo*(N,N-*diethyldithiocarbamato*-S,S')*molybdenum*(V)]

[55723-33-6]



M 584.5

Mo—Mo 277.4 pm. Synth. from $Mo_2O_3(S_2CNEt_2)_2$ and H_2S in CH_2Cl_2. Yellow cryst. (CH_2Cl_2/MeOH).

[69779-02-8]

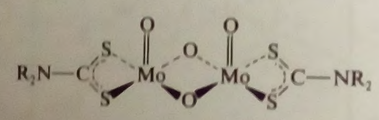
De Hayes, L.J. *et al, Inorg. Chem.*, 1975, **14**, 2110 (*synth, electrochem*)
Nahamura, A. *et al, J. Mol. Catal.*, 1980, **8**, 353 (*catalysis*)
Müller, A. *et al, Z. Anorg. Allg. Chem.*, 1981, **472**, 69 (*synth*)
Lin Chichang, *et al, Jiegou Huaxue*, 1985, **4**, 133 (*cryst struct*)

$C_{10}H_{20}Mo_2N_2O_4S_4$ IC-007079

Bis(*N,N*-diethyldithiocarbamato)di-μ-oxodioxodimolybdenum(*V*)

Bis(diethylcarbamodithioato-S,S')*di-μ-oxodioxodimolybdenum*(V), *11CI, 10CI, 9CI. Di-μ-oxobis[oxodiethyldithiocarbamatomolybdenum*(V)]

[50860-31-6]



R = Et

M 552.4

Struct. comprises two square pyramids sharing an edge. Yellow cryst.

[55780-89-7, 64137-85-5]

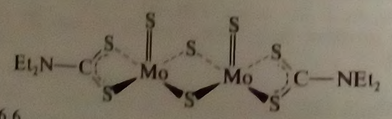
Ricard, L. *et al, Inorg. Chem.*, 1975, **14**, 2300 (*cryst struct, synth*)
Schultz, F.A. *et al, Inorg. Chem.*, 1978, **17**, 1758 (*synth, reactions*)

$C_{10}H_{20}Mo_2N_2S_8$ IC-007080

Bis(*N,N*-diethyldithiocarbamato)di-μ-sulfidodisulfidodimolybdenum(*V*)

Bis(diethylcarbamodithioato-S,S')*di-μ-thioxodithioxodimolybdenum*(V), *11CI. 10CI,9CI. Di-μ-sulfidobis*[(N,N-*diethyldithiocarbamato*)*thiomolybdenum*(V)]

[36539-27-2]



M 616.6

Struct. consists of two square pyramids sharing edge; terminal Mo=S is analogous to molybdenyl Mo=O. Interatomic distances: Mo—Mo 281.7, Mo=S_{av} 209.9 pm. Useful in extreme pressure lubricants; S-ligation may resemble that in nitrogenase. Dark red cryst. (CH_2Cl_2/pentane). Sl. sol. CH_2Cl_2, DMF. Diamagnetic.

[67814-43-1]

Schultz, F.A. *et al, Inorg. Chem.*, 1978, **17**, 1758 (*synth, electrochem*)
Huneke, J.T. *et al, Inorg. Chem.*, 1978, **17**, 3698 (*cryst struct*)

Müller, A. *et al, Z. Anorg. Allg. Chem.*, 1979, **454**, 118 (*cryst struct, ir, synth, uv*)
Halbert, T.R. *et al, Organometallics*, 1985, **4**, 1689 (*reactions*)
Nagaraja, K.S. *et al, Polyhedron*, 1985, **4**, 649.
Nagaraja, K.S. *et al, Transition Met. Chem.*, 1986, **11**, 217 (*synth*)

$C_{10}H_{20}N_2NiO_4S_2$ IC-007081

Bis(methioninato)nickel(*II*)

Bis(DL-*methioninato*-N,O)*nickel, 11CI*

[92078-03-0]

$Ni[OOCCH(NH_2)CH_2CH_2SCH_3]_2$

M 355.1

Uv and props. indicate that struct. is polymeric with octahedrally coordinated Ni and $COO^{\ominus}$ group acting as a bidentate bridging ligand. Synth. from DL-methionine, Na_2CO_3 and $Ni(NO_3)_2.6H_2O$. Light blue air-stable solid. Insol. all solvs. Mp >300°. μ_{eff} = 3.25μ_B.

[14267-16-4, 41579-58-2]

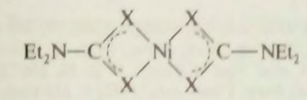
McAuliffe, C.A. *et al, Inorg. Chem.*, 1966, **5**, 1996 (*synth, ir, uv*)
Best, S.A. *et al, Inorg. Chem.*, 1977, **16**, 1976 (*pe*)

$C_{10}H_{20}N_2NiS_4$ IC-007082

Bis(*N,N*-diethyldithiocarbamato)nickel(*II*)

Bis(diethylcarbamodithioato-S,S')*nickel*(II), *9CI*

[14267-17-5]



X = S

M 355.2

Square planar. Dark-brown prisms ($CHCl_3$).

[52610-81-8]

Bonamico, M. *et al, Acta Crystallogr.*, 1965, **19**, 619 (*cryst struct*)
Nanjo, M. *et al, J. Inorg. Nucl. Chem.*, 1970, **32**, 2411 (*props, pmr, ir, uv*)
Golding, R.M. *et al, Aust. J. Chem.*, 1972, **25**, 2567 (*ir, pmr*)
Tavlaridis, A. *et al, Fresenius' Z. Anal. Chem.*, 1978, **293**, 211 (*synth, props*)
Gregor, I.K. *et al, Org. Mass Spectrom.*, 1982, **17**, 575 (*ms*)
Tetsumi, T. *et al, Polyhedron*, 1986, **5**, 707 (*synth, pmr*)

$C_{10}H_{20}N_2NiSe_4$ IC-007083

Bis(*N,N*-diethyldiselenocarbamato)nickel(*II*)

Bis(diethylcarbamodiselenoato-Se,Se')*nickel*(II), *9CI*

[19400-59-0]

As Bis(*N,N*-diethyldithiocarbamato)nickel(*II*), IC-007082 with

X = Se

M 542.8

Green and dark-red (pleochroic) cryst. Sol. C_6H_6, xylene, DMF, $CHCl_3$. Mp 278° ($CHCl_3$) (256°).

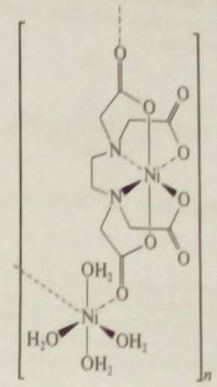
Jensen, K.A. *et al, Acta Chem. Scand.*, 1967, **21**, 2904 (*synth, uv*)
Furlani, C. *et al, Inorg. Chem.*, 1968, **7**, 265 (*synth, uv*)
Bonamico, M. *et al, J. Chem. Soc. A*, 1971, 264 (*cryst struct*)
Pan, W.-H. *et al, J. Am. Chem. Soc.*, 1978, **100**, 5783.
Pan, W.-H. *et al, Inorg. Chem.*, 1981, **20**, 856 (*pmr*)

$C_{10}H_{20}N_2Ni_2O_{12}$ IC-007084

Tetraaqua(ethylenediaminetetraacetato)dinickel(*II*)

Tetraaqua[μ-[[N,N'-*1,2-ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](4−)]]*dinickel*(II), *11CI*

[99687-31-7]



M 477.6

Also known with mixed metals. Synth. from Hexaaquanickel(*II*)(2+), IC-019897 + H_4 edta. Air-stable cryst. + $2H_2O$ (EtOH aq.). Antiferromagnetic.

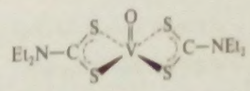
Escrivá, E. *et al, Transition Met. Chem.*, 1984, **9**, 184 (*synth, ir, uv, struct, tga*)
Coronado, E. *et al, J. Am. Chem. Soc.*, 1986, **108**, 900 (*cryst struct, magnetism*)

$C_{10}H_{20}N_2OS_4V$ IC-007085

Bis(*N,N*-diethyldithiocarbamato)oxovanadium(*IV*)

Bis(diethylcarbamodithioato-S,S')*oxovanadium*(IV), *11CI*

[15283-34-8]



M 363.4

Synth. by adding a soln. of $VO(SO_4)$ in aq. EtOH to Na salt of ligand in EtOH. Blue-grey solid with pink dichroism. Sol. $CHCl_3$.

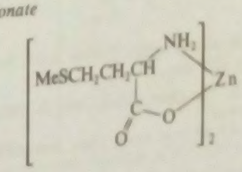
[35944-45-7]

Henrick, K. *et al, J. Chem. Soc., Dalton Trans.*, 1976, 26 (*synth, cryst struct*)
Jezierski, A. *et al, J. Chem. Soc., Dalton Trans.*, 1981, 1 (*esr, reaction*)

$C_{10}H_{20}N_2O_4S_2Zn$ IC-007086

Bis(methionato)zinc

Zinc methionate



M 361.8

L-form [40816-51-1]
Colourless plates.

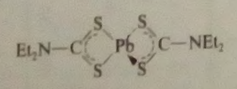
DL-form [64364-41-6]
Mp >360°.

[39358-60-6]

Akihama, S. *et al*, *Chem. Pharm. Bull.*, 1962, **10**, 1254 (*synth*)
Wilson, R.B. *et al*, *Inorg. Chem.*, 1977, **16**, 1498 (*cryst struct*)

$C_{10}H_{20}N_2PbS_4$ IC-007087

Bis(*N,N*-diethyldithiocarbamato)lead(*II*)
Bis(diethylcarbamodithioato-S,S′)lead. Lead(II) *diethyldithiocarbamate*
[17549-30-3]



M 503.7
Synth. from $Pb(OAc)_2$ + Et_2NCS_2Na. Prisms (Et_2O).

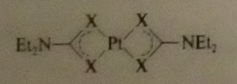
▷ EZ5600000.

[6901-79-7]

Ito, T., *Acta Crystallogr., Sect. B*, 1972, **28**, 1034 (*cryst struct*)
Chang, H.P. *et al*, *Spectrosc. Lett.*, 1981, **14**, 795 (*synth, pe*)
Riekkola, M.-L., *Acta Chem. Scand., Ser. A*, 1983, **37**, 691 (*ms*)
Kellner, R. *et al*, *Mikrochim. Acta*, 1983, **III**, 183 (*far-ir, raman*)
Kellner, R. *et al*, *Inorg. Chim. Acta*, 1984, **84**, 233 (*ir*)

$C_{10}H_{20}N_2PtS_4$ IC-007088

Bis(*N,N*-diethyldithiocarbamato)platinum(*II*), 8Cl
Bis(diethylcarbamodithioato-S,S′)platinum, 9Cl
[15730-38-8]



X = S

M 491.6
Square planar struct. Most accessible dithiocarbamate of Pt. Yellow prisms. Sol. CH_2Cl_2; sl. sol. $CHCl_3$. Mp 245-250°.

Amanov, A.Z. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1967, **8**, 149 (*struct*)
Alison, J.M.C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 254 (*synth, pmr*)
Gaal, H.L.M. *et al*, *Inorg. Chem.*, 1979, **18**, 3251 (*cmr*)
Riekkola, M.L. *et al*, *Acta Chem. Scand., Ser. A*, 1983, **37**, 691 (*ms*)
Colton, R. *et al*, *Polyhedron*, 1984, **3**, 23 (*Pt-195 nmr*)

$C_{10}H_{20}N_2PtSe_4$ IC-007089

Bis(*N,N*-diethyldiselenocarbamato)platinum(*II*), 8Cl
Bis(diethylcarbamodiselenato-Se,Se′)platinum, 10Cl
[19400-65-8]

As Bis(*N,N*-diethyldithiocarbamato)platinum(*II*), IC-007088 with

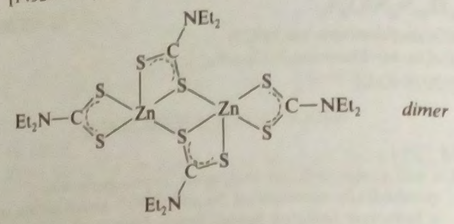
X = Se

M 679.2
Probable square planar struct. Yellow solid. Sol. $CHCl_3$, Me_2CO. Mp 300° dec.

Jensen, K.A. *et al*, *Acta Chem. Scand.*, 1967, **21**, 2904; 1970, **24**, 743 (*synth, uv-vis*)
van der Linden, J.G.M. *et al*, *Inorg. Chim. Acta*, 1979, **35**, 65 (*electrochem*)

$C_{10}H_{20}N_2S_4Zn$ IC-007090

Bis(*N,N*-diethyldithiocarbamato)zinc
Bis(N,N*-diethyldithiocarbamodithioato-*S,S'*)zinc, 9Cl. Zinc diethyldithiocarbamate*
[14324-55-1]



dimer

M 361.9
Dimeric in solid state with distorted trigonal bipyramidal Zn. Vulcanisation accelerator, antioxidant (for polymers); used in epitaxy of ZnS; fungicide and bactericide (antifouling agent). Subl. >130°. Dec. at 230° via $Zn_2(SCSNEt_2)_2$.

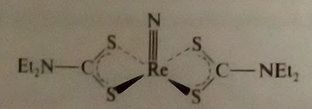
▷ ZH0350000.

Dimer: Bis[μ-(diethylcarbamodithioato-S,S′:S)] bis(diethylcarbamodithioato-S,S′)dizinc
$C_{20}H_{40}N_4S_8Zn_2$ M 723.8
Air-stable pale yellow cryst. ($Me_2CO/CHCl_3$). Mp 177-179° (184°).

Bonamico, M. *et al*, *Acta Crystallogr.*, 1965, **19**, 898 (*cryst struct*)
Coucouvanis, D., *Prog. Inorg. Chem.*, 1970, **11**, 233.
Golding, R.M. *et al*, *Aust. J. Chem.*, 1972, **25**, 2567 (*pmr*)
Villa, J.F. *et al*, *Inorg. Chim. Acta*, 1972, **6**, 332 (*ms*)
Cauletti, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1068 (*pe*)
Yamazaki, M. *et al*, *Nippon Kagaku Kaishi* (*J. Chem. Soc. Jpn.*), 1980, 1723; *CA*, **94**, 57426 (*pmr, cmr*)
Riekkola, M.L., *Acta Chem. Scand., Ser. A*, 1983, **37**, 691 (*ms*)
Lakuda, J. *et al*, *Chem. Zvesti*, 1983, **37**, 733; 1984, **38**, 597 (*stability const*)
Kellner, R. *et al*, *Mikrochim. Acta*, 1983, **3**, 183 (*ir, raman*)
Granozzi, G. *et al*, *Inorg. Chem.*, 1984, **23**, 702 (*pe*)
Kellner, R. *et al*, *Inorg. Chim. Acta*, 1984, **84**, 233 (*ir, raman*)
Geloso, C. *et al*, *Can. J. Chem.*, 1987, **65**, 928 (*synth*)
Skachkov, B.K. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1988, **302**, 1149 (*thermal anal*)
Oleinik, S.P. *et al*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1989, **307**, 1411 (*thermal dec*)

$C_{10}H_{20}N_3ReS_4$ IC-007091

Bis(*N,N*-diethyldithiocarbamato)nitridorhenium(*V*)
Bis(diethylcarbamodithioato-S,S'*)nitridorhenium*(V), *9Cl*
[36472-83-0]

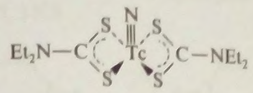


M 496.7
Interatomic distances: Re≡N 168.9, Re—S (av.) 238.9 pm; angle: NReS 108°. Synth. from $ReNCl_2(PPh_3)_2$ and Na salt of ligand in Me_2CO. Yellow cryst. (Me_2CO).

Fletcher, S.R. *et al*, *J. Chem. Soc., Chem. Commun.*, 1970, 1572 (*cryst struct*)
Rowbottom, J.E. *et al*, *J. Chem. Soc., Dalton Trans.*, 1972, 826 (*synth, ir, props*)

$C_{10}H_{20}N_3S_4Tc$ IC-007092

Bis(*N,N*-diethyldithiocarbamato)nitridotechnetium(*V*)
Bis(diethylcarbamodithioato-S,S'*)nitridotechnetium*(V), *11Cl. Tc-99m-DDC*
[77933-43-8]



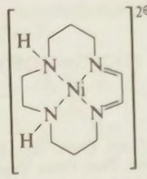
M 409.4
Square-pyramidal. Synth. from $TcNCl_2(PPh_3)_2$ and $Na[S_2CNEt_2]$ in Me_2CO; or from $TcO_4^{\ominus}$, $N_2H_4H_2O$, NaOH, and $Na[S_2CNEt_2]$ in H_2O. Proposed for brain imaging. Yellow solid. Sol. $CHCl_3$. Mp 255°.

[79873-74-8]

Kaden, L. *et al*, *Isotopenpraxis*, 1981, **17**, 174 (*synth, ir, pmr*)
Baldas, J. *et al*, *J. Chem. Soc., Dalton Trans.*, 1981, 1798 (*synth, cryst struct, ir*)
Abram, U. *et al*, *Inorg. Chim. Acta*, 1984, **94**, L3 (*ir, uv, pmr, analogues*)
Baldas, J. *et al*, *Inorg. Chem.*, 1986, **25**, 150 (*synth*)
Ballinger, J.R. *et al*, *Appl. Radiat. Isot.*, 1987, **38**, 665 (*partition coeff, pharmacol*)
Abram, U. *et al*, *Z. Anorg. Allg. Chem.*, 1987, **544**, 167 (*synth, ir, uv, pmr*)

$C_{10}H_{20}N_4Ni^{2\oplus}$ IC-007093

(1,4,8,11-Tetraazacyclotetradeca-1,3-diene)nickel(*II*)(2+)



M 254.9 (ion)
Suggested intermed. in synth. of (1,4,8,11-Tetraazacyclotetradecane)nickel(*II*)(2+), IC-007157. Not isol.

Inorg. Synth., 1976, **16**, 220.

$C_{10}H_{20}N_4O_2S_4W$ IC-007094

Bis(*N,N*-diethyldithiocarbamato)dinitrosyltungsten
Bis(diethylcarbamodithioato-S,S'*)dinitrosyltungsten, 11Cl. 10Cl, 9Cl*
[39872-71-4]

As Bis(*N,N*-dimethyldithiocarbamato)dinitrosyltungsten, IC-005155 with

R = Et

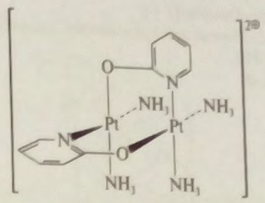
M 540.4
Monomeric, octahedral complex.

cis-form
Synth. from Dibromodinitrosyltungsten, IC-001846 and excess sodium diethyldithiocarbamate. Green needles (MeOH). Sol. org. solvs. Mp >300°. $Subl._{0.01}$ 150°. Diamagnetic.

Johnson, B.F.G., *J. Chem. Soc. A*, 1969, 1668 (*nmr, ir, cryst struct*)
Johnson, B.F.G. *et al*, *Transition Met. Chem.*, 1978, **3**, 81 (*reactions*)
Broomhead, J.A. *et al*, *Aust. J. Chem.*, 1979, **32**, 1187 (*reactions*)
Budge, J.R. *et al*, *Inorg. Chem.*, 1982, **21**, 1031 (*electrochem, esr*)

$C_{10}H_{20}N_6O_2Pt_2^{2\oplus}$ IC-007095

Tetraamminebis[μ-(2(1*H*)-pyridinonato-N^1:O^2)] diplatinum(2+), 1ICl
Tetraamminebis(α-pyridonato)diplatinum(II)(2+)
[76775-75-2]



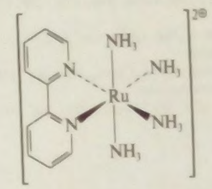
M 646.4 (ion)
Head-to-tail form only stereoisomer known.

Dinitrate: [85336-85-2].
Synth. from eg. *cis*-$[Pt(NH_3)_2(NO_3)_2]$, α-pyridinol and HNO_3. Pale yellow cryst. + $2H_2O$. Equal amounts of both optical isomers in cryst. lattice.

Hollis, L.S. *et al*, *J. Am. Chem. Soc.*, 1983, **105**, 3494 (*synth, cryst struct, pmr, uv, deriv*)

$C_{10}H_{20}N_6Ru^{2\oplus}$ IC-007096

Tetraammine(2,2′-bipyridine-N_1,N')ruthenium(*II*)(2+), 9Cl
[54194-87-5]



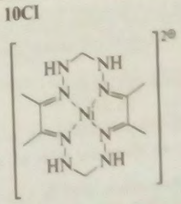
M 325.3 (ion)
Prepd. by treating *cis* Tetraamminedi(aqua)ruthenium(*II*) (2+), IC-019965 with bipy.

Bis-tetrafluoroborate: [54194-88-6].
Solid + $1H_2O$. Sol. H_2O.

Alvarez, V.E. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 7686 (*synth, electrochem, uv*)

$C_{10}H_{20}N_8Ni^{2\oplus}$ IC-007097

(6,7,13,14-Tetramethyl-1,2,4,5,8,9,11,12-octaazacyclotetradeca-5,7,12,14-tetraene-N^1,N^4,N^8,N^{11}) nickel(*II*)(2+), 10Cl



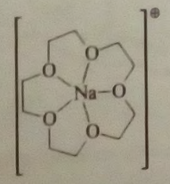
M 311.0 (ion)
Formed by template reaction of $Ni^{2\oplus}$, H_2CO and 2,3-butanedione dihydrazone. Readily dehydrogenated, deprotonated.

Diperchlorate: [60086-90-0].
$C_{10}H_{20}Cl_2N_8NiO_8$ M 509.9

Red-brown solid. Sol. MeCN.
▷ Potentially explosive.
Peng, S.M. *et al, Inorg. Chem.*, 1978, **17**, 119 (*synth, ir, uv, pmr*)

IC-007098

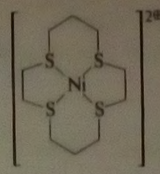
$C_{10}H_{20}NaO_5^{\oplus}$
(15-Crown-5)sodium(1+)
1,4,7,10,13-Pentaoxacyclopentadecane, sodium(1+) complex, 9CI
[59890-71-0]



M 243.2 (ion)
Formed by the reaction of a sodium salt with 15-crown-5 in MeOH.
Thiocyanate: Sodium thiocyanate 15-crown-5 complex Cryst. $Na^{\oplus}$ lies within the plane formed by the crown heteroatoms.
Ethylacetoacetate enolate: Cryst. $Na^{\oplus}$ lies above the plane formed by the crown heteroatoms (~105 pm) and its coordn. sphere is completed by an anion.
Groth, P., *Acta Chem. Scand., Ser. A*, 1981, **35**, 721 (*cryst struct, thiocyanate*)
Dale, L.J. *et al, J. Am. Chem. Soc.*, 1981, **103**, 3773 (*Na-23 nmr, cmr*)
Nakamura, T. *et al, Bull. Chem. Soc. Jpn.*, 1982, **55**, 1850 (*thermodynamics*)
Cambillau, C. *et al, Can. J. Chem.*, 1982, **60**, 2554 (*cryst struct, ethylacetoacetate enolate*)
Takeuchi, H. *et al, J. Mol. Struct.*, 1986, **146**, 197 (*raman, conform*)

IC-007099

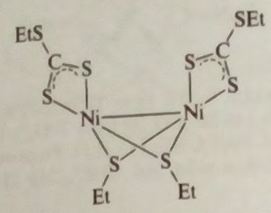
$C_{10}H_{20}NiS_4^{2\oplus}$
(1,4,8,11-Tetrathiacyclotetradecane-S^1,S^4,S^8,S^{11})nickel(II)(2+), 8CI
[46365-94-0]



M 327.2 (ion)
Best studied complex of a macrocyclic ligand with 4S donors. BF_4, ClO_4 salts are square planar, others octahedral.
Bis-tetrafluoroborate: [25460-51-9].
$C_{10}H_{20}B_2F_8NiS_4$ M 500.8
Orange-red solid. Sol. $MeNO_2$.
Rosen, W. *et al, J. Am. Chem. Soc.*, 1969, **91**, 4694 (*synth, ir, uv, elec cond*)
Davis, P.H. *et al, Inorg. Chem.*, 1975, **14**, 1753 (*cryst struct*)
Smith, G.F. *et al, J. Chem. Soc., Chem. Commun.*, 1975, 807.
Herron, N. *et al, Inorg. Chim. Acta*, 1976, **20**, L43 (*cmr*)

IC-007100

$C_{10}H_{20}Ni_2S_8$
Bis[μ-(ethanethiolato)]bis(monoethylcarbonotrithioato-S',S'')dinickel(II), 9CI
Bis(μ-ethanethiolato)bis(hydrogentrithiocarbonato)nickel, diethyl ester, 8CI. Bis(ethanethiolato)bis(ethylthioxanthato) dinickel(II)
[15283-35-9]



M 514.1
Wedge-shaped struct. with sq. planar coordination of S atoms to Ni and Ni-Ni interaction. Synth. from $CS_3Et^{\ominus}$, $EtS^{\ominus}$ and $NiCl_2$ and by attempted crystallisation of $(CS_3Et)_2Ni$. Green cryst. (Me_2CO aq.). Mp 88-90°.
[31233-40-6]
Chiesi Villa, A. *et al, J. Chem. Soc., Chem. Commun.*, 1970, 1322 (*cryst struct*)
Andrews, J.M. *et al, Inorg. Chem.*, 1972, **11**, 493 (*synth, props, uv*)

IC-007101

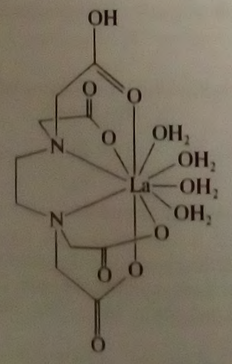
$C_{10}H_{20}O_4$
Tetraethoxyethene, 9CI
Tetraethoxyethylene
[40923-93-1]

$$(EtO)_2C{=}C(OEt)_2$$

M 204.2
Bp_{15} 77°. n_D^{25} 1.4212.
McElvain, S.M. *et al, J. Am. Chem. Soc.*, 1947, **69**, 2661 (*synth*)
Scheeren, J.W. *et al, Recl. Trav. Chim. Pays-Bas (J. R. Neth. Chem. Soc.)*, 1973, **92**, 11 (*synth*)

IC-007102

$C_{10}H_{21}LaN_2O_{12}$
Tetraaqua[[*N*,*N*′-1,2-ethanediylbis[*N*-(carboxymethyl)glycinato]](3−)-*N*,*N*′,*O*,*O*′,O^N,$O^{N'}$]lanthanum(III), 9CI
Tetraaqua(hydrogen ethylenediaminetetraacetato) lanthanum(III)
[11138-89-9]

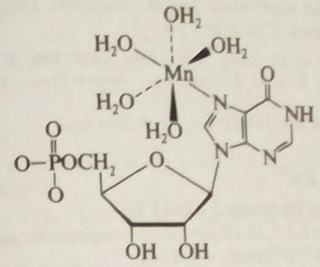


M 500.1
10-Coord. Colourless monoclinic cryst. $+3H_2O$. Sol. H_2O.
[35397-83-2]
Brintzinger, H. *et al, Z. Anorg. Allg. Chem.*, 1943, **251**, 285 (*synth*)
Lind, M.D. *et al, J. Am. Chem. Soc.*, 1965, **87**, 1611 (*synth, cryst struct*)

Martynenko, L.I. *et al, Zh. Neorg. Khim.*, 1972, **17**, 98 (*synth;sRuss. J. Inorg. Chem. (Engl. Transl.)*, 1972, **17**, 51 (*synth*)

IC-007103

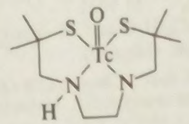
$C_{10}H_{21}MnN_4O_{13}P$
Pentaaqua[inosinato(2−)-5′-monophosphate-N^7]manganese(II), 11CI
[106796-17-2]



M 491.2
Synth. from $Mn(NO_3)_2.6H_2O$ and the disodium salt of inosine 5′-monophosphate. Colourless cryst. + $2H_2O$ (H_2O).
Capparelli, M.V. *et al, Inorg. Chim. Acta*, 1986, **125**, L47 (*synth, cryst struct*)

IC-007104

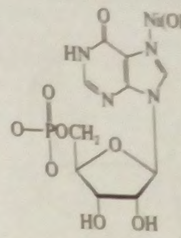
$C_{10}H_{21}N_2OS_2Tc$
[[1,1′-[1,2-Ethanediyl]diimino]bis[2-methyl-2-propanethiolato]](3−)oxotechnetium, 11CI
Tc-BAT-TM. BAT-TM-Tc



M 348.3
Parent of series of pharmacologically important diaminodithiolato-oxo-Tc complexes. Other related complexes include [[1,1′-[[1-(Diethylaminomethylene)-1,2-ethanediyl]diimino]bis[2-methyl-2-propanethiolato]](3−)]oxotechnetium(V), IC-009131, Oxo[[1,1′-[[1-(1-piperidinylmethyl)-1,2-ethanediyl]diimino]bis[2-methyl-2-propanethiolato]](3−)]technetium(V), 12CI, IC-009471 and [1-[[2-[(2-Mercapto-2-methylpropyl)amino]-2-methylpropyl][2-(1-piperidinyl)ethyl]amino]-2-methyl-2-propanethiolato(3−)]oxotechnetium, 12CI, IC-010298. Synth. by $BH_4^{\ominus}$ reduction of $TcO_4^{\ominus}$ + preformed ligand; complex extracted into hexane. Cryst. (EtOH).
Kung, H.F. *et al, J. Nucl. Med.*, 1984, **25**, 326 (*synth, electrophoresis, hplc, partition coeffs, biodistribn*)
Baidoo, K.E. *et al, J. Nucl. Med.*, 1987, **28**, 729 (*partition coeffs, analogues*)

IC-007105

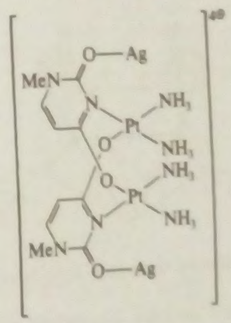
$C_{10}H_{21}N_4NiO_{13}P$
Pentaaqua[inosine-5′-monophosphato(2−)]nickel(II)



M 494.9
Ni coordinated octahedrally with H-bonding between phosphate O, and carbonyl O and ligated water molecules.
Hydrate: Synth. from $Ni(NO_3)_2.6H_2O$ and sodium inosine-5′-monophosphate. Light green cryst. Mp 153-156° dec. $\mu_{eff} = 3.13\mu_B$ (293K).
Nelson, H.G. *et al, Inorg. Chim. Acta*, 1979, **32**, L51 (*synth, uv, hydrate*)

IC-007106

$C_{10}H_{22}Ag_2N_8O_4Pt_2^{4\oplus}$
Tetraamminebis[μ3-(1-methyl-2,4(1*H*,3*H*)-pyrimidinedionato-N^3:O^2:O^4)]bis(silver)diplatinum(4+), 11CI



M 924.2 (ion)
Tetranitrate: [89637-18-3].
Yellow cryst. + $2H_2O$.
Thewalt, U. *et al, Inorg. Chem.*, 1984, **23**, 1713 (*synth, cryst struct, pmr, ir, raman*)

IC-007107

$C_{10}H_{22}AuOPS_2$
***O*-Propyldithiocarbonato(triethylphosphine)gold(I)**
(*O-Propylcarbonodithioato-S,S′*)(*triethylphosphine*)*gold*(I).
(*Propylxanthato*)(*triethylphosphine*)*gold*(I)
As *O*-Methyldithiocarbonato(triethylphosphine)gold(I), IC-006115 with

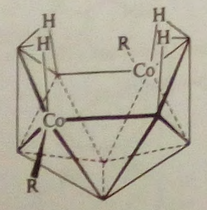
$$R = Et,\ X = OCH_2CH_2CH_3$$

M 450.3
Oil. Mp ~0°. Dec. at 180°.
Kowala, C. *et al, Aust. J. Chem.*, 1986, **39**, 999 (*synth*)

$C_{10}H_{22}B_8Co_2$ IC-007108

Bis(η^5-2,4-cyclopentadien-1-yl)[μ-[η^4:η^4-dodecahydroborato(2−)-*H*,*H*']]dicobalt

[96293-03-7]



R =

M 346.6

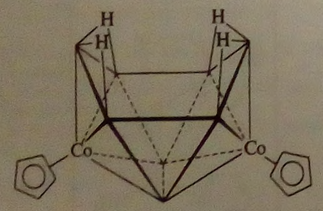
nido. Brown solid (by chromatog. C_6H_6/hexane). Sol. C_6H_6.

Brewer, C.T. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 3552 (*synth, pmr, B-11 nmr, ms, ir*)

$C_{10}H_{22}B_8Co_2$ IC-007109

Bis(η^5-2,4-cyclopentadien-1-yl)[μ-[η^5:η^5-dodecahydrooctaborato(4−)]]dicobalt

[96293-06-0]



M 346.6

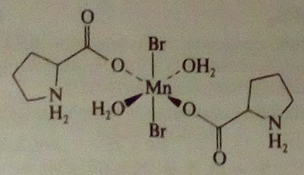
nido-. Yellow solid (by chromatog. C_6H_6/hexane). Sol. C_6H_6.

Brewer, C.T. *et al*, *J. Am. Chem. Soc.*, 1985, **107**, 3552 (*synth, pmr, B-11 nmr, ms, ir*)

$C_{10}H_{22}Br_2MnN_2O_6$ IC-007110

Diaquadibromobis(D,L-proline)manganese(*II*)

[65546-04-5]



M 481.0

trans-Octahedral struct. Synth. from aq. solns. of stoichiometric amounts of $MnBr_2$ and DL-proline. Colourless plates (H_2O).

[73837-13-5]

Glowiak, T. *et al*, *Acta Crystallogr., Sect. B*, 1977, **33**, 3237 (*synth, cryst struct*)

Gmelin Handbook Inorg. Chem., Syst. No. 56, 1985, **D4**, 304 (*rev, bibl*)

$C_{10}H_{22}ClO_3V$ IC-007111

Chlorobis(2,2-dimethyl-1-propanolato)oxovanadium(*V*), 11Cl

Chlorobis(neopentoxy)oxovanadium(V)

[68114-31-8]

$VOCl[OCH_2C(CH_3)_3]_2$

M 276.6

Catalyst for alternating polym. of olefins. (Much of the lit. is Chinese). Colourless liq.

Funk, H. *et al*, *Z. Anorg. Allg. Chem.*, 1958, **296**, 36 (*synth*)

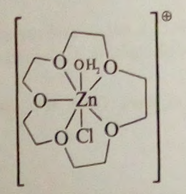
Choukroun, R. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 1800 (*reaction*)

Eur. Pat., 48 844, (1982); *CA*, **97**, 56391g (*use*)

$C_{10}H_{22}ClO_6Zn^{\oplus}$ IC-007112

Aquachloro(15-crown-5)zinc(1+)

Aquachloro(1,4,7,10,13-pentaoxacyclopentadecane-O^1,O^4,O^7,O^{10},O^{13})zinc(1+), 12Cl



M 339.1 (ion)

Pentagonal bipyramidal cation with equatorial 15-crown-5.

Di-μ-chlorotetrachlorodizincate(2−) (2:1): [124023-98-9].

$C_{20}H_{44}Cl_8O_{12}Zn_4$ M 1021.7

Prepd. from $ZnCl_2.H_2O$ and 15-crown-5 in Me_2CO. Light yellow cryst. (Me_2CO).

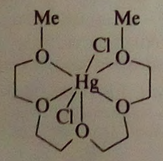
Ivakina, L.V. *et al*, *J. Struct. Chem. USSR* (*Engl. Transl.*), 1989, **30**, 161 (*synth, cryst struct*)

$C_{10}H_{22}Cl_2HgO_5$ IC-007113

Dichloro(2,5,8,11,14-pentaoxapentadecane-*O*,*O*',*O*'',*O*''',*O*'''')mercury(*II*), 9Cl

Dichloro(1,12-dimethoxy-3,6,9-trioxadodecane)mercury. Dichloro(tetraethyleneglycol dimethyl ether)mercury(II). *Dichloro(tetraglyme)mercury*(II). *Mercury*(II) *chloride tetraglyme*

[40802-28-6]



M 493.7

Cryst. (EtOH). Mp 66°.

Iwamoto, R., *Bull. Chem. Soc. Jpn.*, 1973, **46**, 1114 (*synth, cryst struct*)

Wulfsberg, G. *et al*, *Inorg. Chem.*, 1976, **15**, 1791 (*Cl-35 nqr*)

Wulfsberg, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 1640 (*ir, raman*)

Wulfsberg, G. *et al*, *Ber. Bunsenges. Phys. Chem.*, 1980, **84**, 474 (*Cl-35 nqr*)

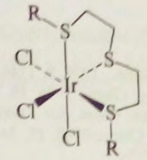
Tabeta, R. *et al*, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 3215 (*cmr*)

$C_{10}H_{22}Cl_3IrS_3$ IC-007114

Trichloro(4,7,10-trithiatridecane)iridium(*III*)

[*Bis*[2-(*propylthio*)*ethyl*] *sulfide*]*trichloroiridium*(III), *8Cl*

[31842-44-1]



R = $CH_2CH_2CH_3$

M 537.0

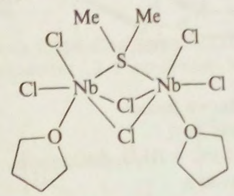
Probably *fac*-config. Yellow solid. Sol. 1,2-dichloroethane. Mp 190-192°.

Chatt, J. *et al*, *J. Chem. Soc. A*, 1971, 899 (*synth, ir*)

$C_{10}H_{22}Cl_6Nb_2O_2S$ IC-007115

Di-μ-chlorotetrachloro(μ-dimethylsulfide) bis(tetrahydrofuran)diniobium(*III*)

Di-μ-chlorotetrachlorobis(tetrahydrofuran)[μ-[*thiobis*[*methane*]]]*diniobium*(III), *11Cl. Di-μ-chloro(μ-dimethyl sulfide)bis*[*dichloro*(*tetrahydrofuran*)*niobium*(III)]



M 604.8

Confacial bioctahedral. Synth. by slow diffusion of hexane into a THF soln. of $Nb_2Cl_6(SMe_2)_3$. Red, air-sensitive cryst.

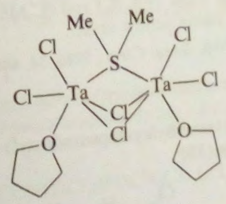
Cotton, F.A. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 878 (*synth, cryst struct*)

$C_{10}H_{22}Cl_6O_2STa_2$ IC-007116

Di-μ-chlorotetrachloro[μ-(dimethyl sulfide)] bis(tetrahydrofuran)ditantalum(*III*)

Di-μ-chlorotetrachlorobis(tetrahydrofuran)[μ-[*thiobis*[*methane*]]]*ditantalum*(III), *11Cl. Di-μ-chloro(μ-dimethyl sulfide)bis*[*dichloro*(*tetrahydrofuran*)*tantalum*(III)]

[97349-08-1]



M 780.9

Bi-octahedral struct. Synth. by slow diffusion of hexane into THF soln. of $Ta_2Cl_6(SMe_2)_3$. Red solid.

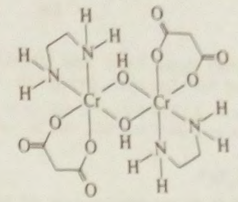
Cotton, F.A. *et al*, *Acta Crystallogr., Sect. C*, 1985, **41**, 878 (*synth, cryst struct*)

$C_{10}H_{22}Cr_2N_4O_{10}$ IC-007117

Bis(ethylenediamine)di-μ-hydroxybis(malonato) dichromium(*III*)

Bis(1,2-ethanediamine-N,N')di-μ-hydroxybis[propanedioato(2−)-O,O']dichromium, *10Cl. Di-μ-hydroxobis[(ethylenediamine)malonatochromium*(III)]

[75675-63-7]



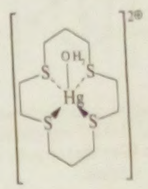
M 462.2

Bioctahedral. Bright red cryst. + $6H_2O$.

Lethbridge, J.W., *J. Chem. Soc., Dalton Trans.*, 1980, 2039 (*cryst struct, synth, uv*)

$C_{10}H_{22}HgOS_4^{2\oplus}$ IC-007118

Aqua(1,4,8,11-tetrathiacyclotetradecane-S^1,S^4,S^8,S^{11}) mercury(2+), 10Cl



M 487.1 (ion)

Tetragonal pyramidal Hg in solid state.

Diperchlorate: [67540-03-8].

White cryst. (aq. MeOH).

▷ Potentially explosive.

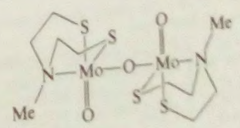
Alcock, N.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1978, 394 (*synth, cryst struct*)

$C_{10}H_{22}Mo_2N_2O_3S_4$ IC-007119

Bis[[2,2'-(Methylimino)bis[ethanethiolato]](2−)-*N*,*S*,*S*']-μ-oxodioxodimolybdenum(*V*), 10Cl

Bis[methyldi(2-mercaptoethyl)aminato(2−)]-μ-oxodioxodimolybdenum(V). *μ-Oxobis[oxo[methyldi(2-thiolatoethyl)amine]molybdenum*(V)]

[67251-57-4]



M 538.4

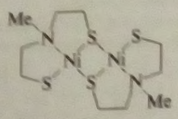
Deep brown, mod. air-stable cryst. (DMSO/EtOH). Spar. sol. with slow dec. DMSO, DMF, HMPA. Ir ν_{MoO} 945s cm^{-1}, ν_{MoOMo} 746m cm^{-1} (KBr).

Tsao, Y.-Y.P. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 4089 (*cryst struct, synth, ir*)

$C_{10}H_{22}N_2Ni_2S_4$ IC-007120

Bis(3-aza-3-methylpentane-1,5-dithiolato)dinickel(*II*)

Bis[di(mercaptoethyl)methylaminato(2−)]dinickel(II)



M 415.9

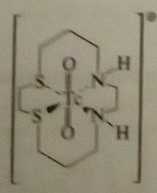
Proposed struct. shown. Synth. from $MeN(CH_2CH_2SH)_2$, $NiSO_4$ and NH_3. Red cryst., diamagnetic. V. sol. $CHCl_3$.

Harley-Mason, J., *J. Chem. Soc.*, 1952, 146 (*synth*)
Busch, D.H. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 3642 (*props*)

$C_{10}H_{22}N_2O_2S_2Tc^{\oplus}$ IC-007121

(1,4-Dithia-8,11-diazacyclotetradecane-N^8,N^{11},S^1,S^4)dioxotechnetium(1+), 12Cl

Dioxo(1,4-dithia-8,11-diazacyclotetradecane)technetium(V) (*1+*)



M 365.3 (ion)

trans-Octahedral cation; macrocyclic analogue of Tc-DADS(BAT) and -DADT complexes with $TcON_2S_2$ core. Cations are H-bonded in pairs in cryst. Synth. from $[TcOBr_4]^{\ominus}$ + ligand.

Hexafluorophosphate: [120661-87-2].
Yellow solid. Sol. H_2O; spar. sol. EtOH.

Ianoz, E. *et al*, *Inorg. Chim. Acta*, 1989, **156**, 235 (*synth, cryst struct, uv, ir*)

$C_{10}H_{22}N_4Ru^{2\oplus}$ IC-007122

Tetraamminebis(pyridine)ruthenium(*II*)(2+), 9Cl

$[Ru(NH_3)_4(Py)_2]^{2\oplus}$

M 327.3 (ion)

Pseudo-octahedral. Prepd. by treating the appropriate isomer of Tetraammined(aqua)ruthenium(*II*)(2+), IC-019965 with Py. Sol. H_2O.

cis-form [46751-30-8]

Diperchlorate: Yellow cryst.

trans-form [46751-29-5]

Diperchlorate: Yellow cryst.

Allen, A.D. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 5595 (*synth*)
Ford, P.C. *et al*, *Inorg. Chem.*, 1969, **8**, 1544 (*synth, uv*)
Zwickel, A.M. *et al*, *Inorg. Chem.*, 1971, **10**, 2395 (*uv, theory*)
Lavallee, D.K. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2583; 1977, **99**, 718 (*pmr, cmr*)
Chaisson, D.A. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 6665 (*synth, uv*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*electrochem*)

$C_{10}H_{22}N_4Ru^{3\oplus}$ IC-007123

Tetraamminebis(pyridine)ruthenium(*III*)(3+), 9Cl

[74497-52-2]

$[Ru(NH_3)_4(Py)_2]^{3\oplus}$

M 327.3 (ion)

Pseudo-octahedral. Synth. by the oxidation of the appropriate isomer of Tetraamminebis(pyridine) ruthenium(*II*)(2+), IC-007122 with acidic H_2O_2. Soln. species. Sol. H_2O.

cis-form [58560-95-5]

trans-form [58560-94-4]

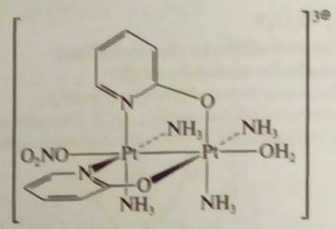
Ford, P.C. *et al*, *Inorg. Chem.*, 1969, **8**, 1544 (*synth, uv*)
Matsubara, T. *et al*, *Inorg. Chem.*, 1976, **15**, 1107 (*electrochem*)
Diamond, S.E. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 5908 (*reaction*)
Bento, M.L. *et al*, *Inorg. Chem.*, 1988, **27**, 3410 (*uv, electrochem, trans-form*)

$C_{10}H_{22}N_7O_6Pt_2^{3\oplus}$ IC-007124

Tetraammineaqua(nitrato-*O*)bis[μ-(2(1*H*)-pyridinonato-N^1:O^2)]diplatinum(3+), 11Cl

Tetraammine(aqua)nitratobis(α-pyridonato)diplatinum(3+)

[86308-20-5]



M 726.4 (ion)

cis-form only known isomer.

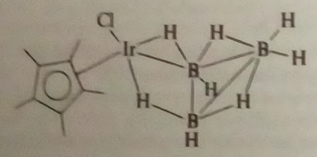
Trinitrate: [86308-22-7].
Red-orange cryst. $+2H_2O$, diamagnetic.

[79745-48-5, 79745-50-9]

Hollis, L.S. *et al*, *Inorg. Chem.*, 1983, **22**, 2605 (*synth, uv, cryst struct*)

$C_{10}H_{23}B_3ClIr$ IC-007125

2-Chloro-2-(pentamethylcyclopentadienyl)-2-iridatetraborane(10)



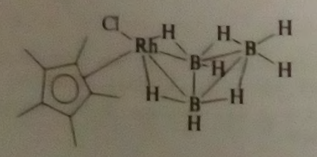
M 403.3

arachno-. Synth. from $Tl[B_3H_8]$ and $(C_5Me_5)IrCl_2$ in CH_2Cl_2. Air stable yellow cryst.

Kennedy, J.D., *Prog. Inorg. Chem.*, 1986, **34**, 406 (*synth*)

$C_{10}H_{23}B_3ClRh$ IC-007126

2-Chloro-2-(pentamethylcyclopentadienyl)-2-rhodatetraborane(10)



M 314.0

arachno-. Synth. from $Tl[B_3H_8]$ and $(C_5Me_5)RhCl_2$ in CH_2Cl_2. Air stable yellow cryst.

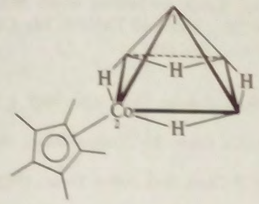
Kennedy, J.D., *Prog. Inorg. Chem.*, 1986, **34**, 406.

$C_{10}H_{23}B_4Co$ IC-007127

2-[(π-Pentamethylcyclopentadienyl)cobalt]pentaborane(9)

[Octahydrotetraborato(1−)][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]cobalt, 11Cl

[80127-20-4]



M 245.4

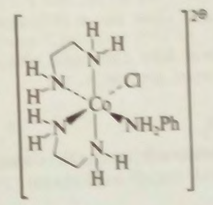
nido. Air-stable red-orange cryst. (CH_2Cl_2/hexane by chromatog.). Sol. CH_2Cl_2, $CHCl_3$. Mp 92-94°.

Venable, T.L. *et al*, *Inorg. Chem.*, 1982, **21**, 887 (*synth, B-11 nmr, pmr, ir, ms*)

$C_{10}H_{23}ClCoN_5^{2\oplus}$ IC-007128

Anilinechlorobis(ethylenediamine)cobalt(*III*)(2+)

(Benzenamine)chlorobis(1,2-ethanediamine-N,N')cobalt(2+), 9Cl



cis-form

M 307.7 (ion)

Prepd. by reaction of the dichloro analogue with aniline.

cis-form [46753-03-1]

Dichloride: [15079-88-6].
Red-violet cryst.

[15242-45-2]

Bailar, J.C. *et al*, *J. Am. Chem. Soc.*, 1945, **67**, 171 (*synth*)
Yasui, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1963, **36**, 1286 (*ir, uv*)
Buckingham, D.A. *et al*, *Aust. J. Chem.*, 1967, **20**, 257 (*pmr*)

$C_{10}H_{23}Cl_3NO_2Ti$ IC-007129

(Acetonitrile)bis(1-butanol)trichlorotitanium(*III*), 11Cl

Titanium(III) *chloride acetonitrile bis(1-butanol)*

[87052-15-1]

$(H_3CCN)TiCl_3(HOCH_2CH_2CH_2CH_3)_2$

M 343.5

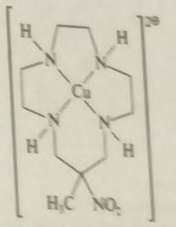
Synth. from $TiCl_3$(MeCN) and 1-butanol. Similar synth. for 2-butanol analogue.

Kohutova, M. *et al*, *Proc. Conf. Coord. Chem.*, 9th, 1983, 169; *CA*, **99**, 114906z (*synth, ir, thermal anal*)

$C_{10}H_{22}CuN_5O_2^{2\oplus}$ IC-007130

(12-Methyl-12-nitro-1,4,7,10-tetraazacyclotridecane-N^1,N^4,N^7,N^{10})copper(*II*)(2+)

[113821-99-1]



M 308.8 (ion)

Diperchlorate: [114367-77-0], *(12-Methyl-12-nitro-1,4,7,10-tetraazacyclotridecane)(perchlorato-O)copper(1+) perchlorate*
Dark red solid. Sol. DMSO, H_2O.
▷ Potentially explosive.

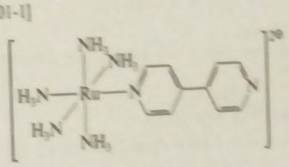
Tetrachlorocuprate(2−): [113822-00-7], *μ-Chlorotrichloro(12-methyl-12-nitro-1,4,7,10-tetraazacyclotridecane)dicopper*(II)
$C_{10}H_{22}Cl_4Cu_2N_5O_2$ M 514.2
Large green cryst.

Comba, P. *et al*, *J. Chem. Soc., Dalton Trans.*, 1988, 497 (*cryst struct, synth, uv, ir*)

$C_{10}H_{22}N_7Ru^{2\oplus}$ IC-007131

Pentaammine(4,4'-bipyridine-*N*)ruthenium(*II*)(2+), 9Cl

[54714-01-1]



M 342.4 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with 4,4'-bipyridine. An important reagent in the formation of complexes containing μ-(4,4'-bipyridine)diruthenium linkages. Sol. H_2O.

Dichloride:
$C_{10}H_{23}Cl_2N_7Ru$ M 413.3
Orange cryst.

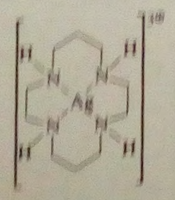
Bis-hexafluorophosphate: Orange-yellow cryst.

Lavallee, D.K. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2583 (*synth, uv, pmr, pK*)
Callahan, R.W. *et al*, *Inorg. Chem.*, 1975, **14**, 1443 (*synth, uv, electrochem*)
Yeh, A. *et al*, *Inorg. Chim. Acta*, 1979, **33**, 51 (*reaction*)
Phillips, J. *et al*, *Inorg. Chem.*, 1980, **19**, 76 (*reaction*)
Moore, K.J. *et al*, *Inorg. Chem.*, 1983, **22**, 1108 (*electrochem*)
Farquharson, S. *et al*, *J. Am. Chem. Soc.*, 1984, **106**, 5123 (*uv, theory*)
Benedix, R. *et al*, *J. Prakt. Chem.*, 1984, **326**, 962 (*uv, photochem, theory*)
Seddon, E.A. *et al*, *The Chemistry of Ruthenium*, Elsevier, Amsterdam, 1984, 331 (*reactions*)
Caswell, D.S. *et al*, *Inorg. Chem.*, 1987, **26**, 18 (*raman*)
Winkler, J.R. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 2381 (*uv*)
Chang, Y.J. *et al*, *Chem. Phys. Lett.*, 1989, **158**, 421 (*photophysics, photochem*)

$C_{10}H_{22}AgN_4^{3\oplus}$ – $C_{10}H_{22}ClHgN_4^{\oplus}$

$C_{10}H_{22}AgN_4^{3\oplus}$ IC-007132

(1,4,8,11-Tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})silver(3+), 9Cl

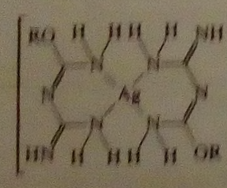


M 308.1 (ion)
Square planar at Ag.
Triperchlorate: [41884-07-5].
Obt. by oxidation of Ag^{II} analogue. Pale yellow cryst. ($MeCN/Et_2O$).
Potentially explosive.

Barnfield, E.K. *et al, Inorg. Chem.*, 1973, **12**, 2829 (*synth, electrochem, magnetism, uv*)

$C_{10}H_{24}AgN_8O_3^{3\oplus}$ IC-007133

Bis(1-amidino-2-isopropylpseudourea)silver(3+), 8Cl



R = $CH(CH_3)_2$

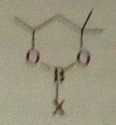
M 396.2 (ion)
High oxidation state, 4 coordinate silver. Tentative struct. shown.
Sulfate (2:3): [11063-82-4].
Orange-brown cryst. (H_2O).

Chatterjee, B. *et al, J. Indian Chem. Soc.*, 1970, **47**, 1021 (*synth, uv*)

$C_{10}H_{24}BClO_4Sn_2$ IC-007134

2-[(3-Chloro-1,1,3,3-tetramethyldistannoxanyl)oxy]-4,4,6-trimethyl-1,3,2-dioxaborinane, 10Cl

[63245-40-9]



X = $-OSnMe_2OSnMe_2Cl$

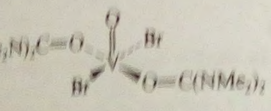
M 491.9
Heat stabiliser for pvc; fungicide. White cryst. Mp 252-253°.

Ger. Pat., 2 703 904, (1977); *CA*, **89**, 44633a (*use*)
U.S. Pat., 4 021 407, (1977); *CA*, **87**, 54075t (*use*)
U.S. Pat., 4 035 403, (1977); *CA*, **87**, 135950b (*use, synth*)
Ger. Pat., 2 718 320, (1978); *CA*, **89**, 24538v (*use, synth*)

$C_{10}H_{24}Br_2N_4O_3V$ IC-007135

Dibromooxobis(tetramethylurea-*O*)vanadium(*IV*), 1Cl

[87900-66-1]



M 459.0
Square pyramidal with *trans*-Br; the chloride is isostructural. Synth. by heating under reflux conc. aq. solns. of $VOBr_2$, HBr and TMU in Me_2CO. Cryst. Sol. MeCN. Ir $\nu_{V=O}$ 992 cm^{-1}.

[16774-79-1]

du Preez, J.G.H. *et al, Inorg. Chim. Acta*, 1967, **1**, 202 (*synth, uv-vis, ir*)
Collison, D. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 667 (*uv-vis, cryst struct*)
Gahan, B. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1695 (*esr*)

$C_{10}H_{24}Br_4N_4O_2U$ IC-007136

Tetrabromobis(tetramethylurea-*O*)uranium(*IV*)

Uranium(IV) *bromide bis(tetramethylurea)*

$UBr_4[O{=}C(NMe_2)_2]_2$

M 789.9
Octahedral.

trans-form [41494-08-0]
Pale blue-green cryst. Sol. CH_2Cl_2, sl. sol. MeCN. Mp 250° dec.

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1971, 2124 (*synth, ir, magnetism*)
du Preez, J.G.H. *et al, Inorg. Chim. Acta*, 1986, **122**, 119; 1987, **129**, 289 (*cryst struct, synth, uv, ir, tga*)

$C_{10}H_{24}CeCl_4N_4O_2$ IC-007137

Tetrachlorobis(tetramethylurea-*O*)cerium(*IV*), 1Cl

Cerium(IV) *chloride bis(tetramethylurea)*

[87800-49-5]

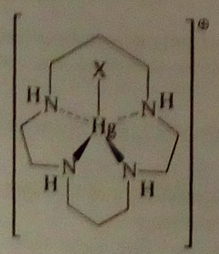
$CeCl_4[O{=}C(NMe_2)_2]_2$

M 514.2
Brick red solid. Sol. CH_2Cl_2. Dec. at *ca.* 180°. Ir ν_{CeCl} 264-243 cm^{-1}.

Barry, J. *et al, J. Chem. Soc., Dalton Trans.*, 1983, 1265 (*synth, ir, dta*)

$C_{10}H_{24}ClHgN_4^{\oplus}$ IC-007138

Chloro(1,4,8,11-tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})mercury(1+)



X = Cl

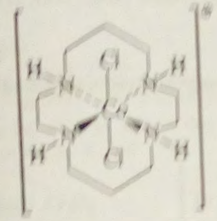
M 436.3 (ion)

Tetrachloromercurate(2−) (2:1): Cryst. Sol. DMSO.
Alcock, N.W. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1987 (*synth, props, ir, cryst struct*)

$C_{10}H_{24}Cl_2CoN_4^{\oplus}$ IC-007139

Dichloro(1,4,8,11-tetraazacyclotetradecane)cobalt(*III*)(1+)
Dichloro(cyclam)cobalt(1+)

[19973-61-6]



trans-form

M 330.1 (ion)

cis-form
Chloride: Purple (violet) cryst. (2*M* HCl). Sol. hot 6*M* HCl (part isom.).

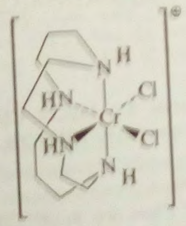
trans-form
On hydrol. affords *trans*-[Co(cyclam)$(OH_2)Cl$]$^{2\oplus}$.
Chloride: Green cryst. Sol. hot H_2O. Also obt. as nitrate and perchlorate salts.

[6684-16-5, 6684-17-6, 6684-18-7]

Bosnich, B. *et al, Inorg. Chem.*, 1965, **4**, 1102 (*synth, trans-form*)
Poon, C.K. *et al, J. Chem. Soc. A*, 1967, 2069; 1968, 1549 (*cis-form, synth, substn, ms, uv-vis*)
Cragel, J. *et al, Inorg. Chim. Acta*, 1974, **10**, 33 (*synth*)
Hung, Y. *et al, J. Am. Chem. Soc.*, 1977, **99**, 4029 (*synth, ir, uv-vis, electrochem*)

$C_{10}H_{24}Cl_2CrN_4^{\oplus}$ IC-007140

Dichloro(1,4,7,11-tetraazacyclotetradecane-N^1,N^4,N^7,N^{11})chromium(*III*)(1+), 1Cl, 1OCl



M 323.2 (ion)
Octahedral cation.

cis-form [101009-49-8]
Red.
Chloride: [78804-42-9].
Dark red solid (aq. HCl/Me_2CO). Insol. MeOH. μ_{eff} = 3.6μ_B (298K).

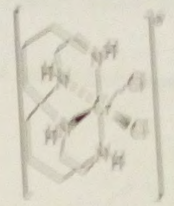
trans-form [101009-51-2]
λ_{max} 582 nm (H_2O).
Chloride: [78854-19-0].
Green solid (aq. Me_2CO). Sol. MeOH. 1:1 electrolyte.
μ_{eff} = 3.6 μ_B (298K).

Swisher, R.G. *et al, Inorg. Chem.*, 1981, **20**, 3947; 1986, **25**, 1320 (*uv-vis, synth, magnetism, conductivity*)

$C_{10}H_{24}Cl_2CrN_4^{\oplus}$ IC-007141

Dichloro(1,4,8,11-tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})chromium(*III*)(1+), 1Cl, 1OCl, 9Cl

Trichloro(cyclam)chromium(1+)



cis-form

M 373.2 (ion)
Legend can be flat or folded leading to trans- or cis-octahedral complexes and config. of coordinated nitrogens (R or S) varies in situ. Important in kinetic and photochemical studies. Electronic and infrared spectra etc. can be used to differentiate between cis- and trans-isomers if x-ray struct. unknown.

cis-form [30051-73-1]
Generally cryst. as racemic mixt. (*RS,RS,RS,RS*), but has been resolved. λ_{max} 529, 464 nm.
Chloride: [27405-95-6].
Refluxing $CrCl_3.3THF$ in DMF with macrocycle gives mainly cis-isomer (~90%). Dark red cryst. (aq. HCl/Me_2CO).
Perchlorate: [27405-97-8].
(−)(*R,R,R,R*)-*form, perchlorate*: [93219-77-3].
Violet cryst. (12*M* HCl/60% $HClO_4$). Cr—Cl 231.1, Cr—N 208.4, 207.6 pm (similar to chloride).

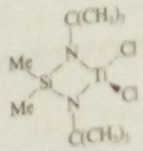
trans-form [30051-74-2]
More difficult to prepare than cis-form. λ_{max} 567, 464sh, 364 nm (values very sl.).
Chloride: [27385-72-4].
trans-form obt. by refluxing aq. cis-form at pH7 for 8h, adding HCl, evapn., and extraction with MeOH. Dark purple needles (1*M* HCl) or grey-green (grey pink in tungsten light) needles (Me_2CO aq.).
Perchlorate: [27385-71-3].
[102491-40-7, 102491-41-8, 102517-42-0, 102517-58-8]

Ferguson, J. *et al, Inorg. Chim. Acta*, 1970, **4**, 109 (*synth, uv-vis*)
Poon, C.K. *et al, Inorg. Chem.*, 1980, **19**, 568 (*improved synth, uv-vis, ir*)
House, D.A. *et al, Inorg. Chem.*, 1984, **23**, 4237 (*cryst struct, cis-perchlorate, synth, ord, cd, uv-vis*)
Forsellini, E. *et al, Acta Crystallogr., Sect. C*, 1986, **42**, 563 (*cryst struct, cis-chloride*)
Sosa, M.E. *et al, J. Chem. Soc., Dalton Trans.*, 1986, 427 (*synth, kinetics*)
Forster, L.S. *et al, J. Phys. Chem.*, 1986, **90**, 5131 (*photochem*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 918 (*rev*)

$C_{10}H_{24}Cl_2N_2SiTi$ IC-007142

[*N,N'*-Bis(1,1-dimethylethyl)-1,1-dimethylsilanediaminato(2−)-*N,N'*]dichlorotitanium(*IV*), 1Cl, 1OCl

[85885-62-7]



M 319.1

Synth. from $TiCl_4$ and the dilithium salt of the ligand in hexane. Lemon-yellow solid. Sol. hexane. Mp 58°.

Burger, H. *et al*, *Z. Anorg. Allg. Chem.*, 1979, **459**, 111 (*synth, ir, raman, pmr*)
Jones, R.A. *et al*, *J. Organomet. Chem.*, 1983, **247**, 1 (*cryst struct*)

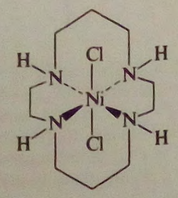
IC-007143

$C_{10}H_{24}Cl_2N_4Ni$

Dichloro(1,4,8,11-tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})nickel(*II*)

Dichloro(cyclam)nickel

[15333-47-8]



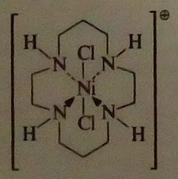
M 329.9
trans-Octahedral. Mauve cryst. Sol. H_2O, MeOH, $PhNO_2$; insol. other org. solvs.

Bosnich, B. *et al*, *Inorg. Chem.*, 1965, **4**, 1109 (*synth, props*)
Bosnich, B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1965, 97 (*cryst struct*)
Martin, L.Y. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 2968 (*uv, pmr*)
Dei, A., *Inorg. Chem.*, 1979, **18**, 891 (*pmr*)
Dei, A., *Inorg. Chim. Acta*, 1982, **65**, L9 (*pmr*)
Ito, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1984, **57**, 1556, 2641 (*cryst struct*)

IC-007144

$C_{10}H_{24}Cl_2N_4Ni^{\oplus}$

Dichloro(1,4,8,11-tetraazacyclotetradecane)nickel(*III*)(1+)



trans-form

M 329.9 (ion)
Macrocyclic ligand stabilises Ni(*III*) in solid state.

trans-form [60105-34-2]

Perchlorate: [60105-35-3].
Yellow cryst., dec. slowly in soln. Sol. H_2O, MeCN, DMSO.

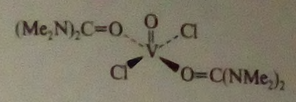
Lovecchio, F.V. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 3109 (*electrochem, esr*)
Chan, P.-K. *et al*, *J. Chem. Soc., Dalton Trans.*, 1976, 858 (*synth, ir, uv*)
Desideri, A. *et al*, *J. Chem. Soc., Dalton Trans.*, 1977, 2051 (*esr*)
Ito, T. *et al*, *Chem. Lett.*, 1981, 1477 (*cryst struct*)

IC-007145

$C_{10}H_{24}Cl_2N_4O_3V$

Dichloroxobis(tetramethylurea-*O*)vanadium(*IV*), 11CI

[16774-78-0]



M 370.1
Square pyramidal. Synth. from $VOCl_2(MeCN)_2$ and tetramethylurea in an org. solv. Blue solid. Sol. $CHCl_3$, $MeNO_2$, MeCN.

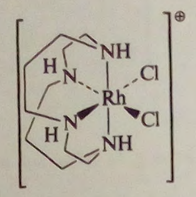
[51017-59-5]

du Preez, J.G.H. *et al*, *Inorg. Chim. Acta*, 1967, **1**, 202 (*synth, ir, uv-vis*)
Coetzer, J., *Acta Crystallogr., Sect. B*, 1970, **26**, 872 (*cryst struct*)
Cave, J. *et al*, *Inorg. Chim. Acta*, 1978, **30**, L349 (*synth, ir, uv-vis*)
Collison, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 667 (*uv-vis*)
Gahan, B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 1695 (*esr*)

IC-007146

$C_{10}H_{24}Cl_2N_4Rh^{\oplus}$

Dichloro(1,4,8,11-tetraazacyclotetradecane)rhodium(*III*)(1+), 8CI



cis-form

M 374.1 (ion)

cis-form

Chloride: [29342-74-3].
Yellow solid. Sol. H_2O.

trans-form

Chloride: [29544-76-1].
Yellow solid. Sol. H_2O.

Bounsall, E.J. *et al*, *Can. J. Chem.*, 1970, **48**, 1481 (*synth, ir, uv*)

IC-007147

$C_{10}H_{24}Cl_4N_4O_2U$

Tetrachlorobis(tetramethylurea-*O*)uranium(*IV*)

Uranium(IV) *chloride bis(tetramethylurea)*

[33337-49-4]

$$UCl_4[O{=}C(NMe_2)_2]_2$$

M 612.1
Octahedral.

trans-form
Pale blue-green cryst. Sol. MeCN, CH_2Cl_2. Mp 250° dec. Dec. begins above 140°. Heating to 300° gives UO_2Cl.

[41494-02-4]

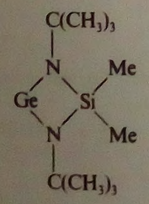
Bagnall, K.W. *et al*, *J. Chem. Soc. A*, 1971, 2124 (*synth, ir, magnetism*)
du Preez, J.G.H. *et al*, *Inorg. Chim. Acta*, 1986, **122**, 119; 1987, **129**, 289 (*synth, uv, cryst struct, tga, ir*)

IC-007148

$C_{10}H_{24}GeN_2Si$

[Dimethylsilylenebis(*tert*-butylimido)-*N*,*N*']germanium

[84806-15-5]



M 273.0
Synth. from $GeCl_2$.dioxan and $Me_2Si(N^tBuLi)_2$.

[36032-85-6]

Peterson, L.K. *et al*, *Can. J. Chem.*, 1972, **50**, 553 (*synth*)
Veith, M. *et al*, *Z. Naturforsch., B*, 1982, **37**, 1375 (*synth*)
Veith, M. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 89 (*reactions*)

IC-007149

$C_{10}H_{24}I_4N_4O_2U$

Tetraiodobis(tetramethylurea-*O*)uranium(*IV*), 12CI

Uranium(IV) *chloride bis(tetramethylurea)*

$$UI_4[O{=}C(NMe_2)_2]_2$$

M 977.9
Octahedral.

trans-form [110548-75-9]
Yellow-green cryst. Sol. Me_2CO.

du Preez, J.G.H. *et al*, *Inorg. Chim. Acta*, 1987, **129**, 289 (*synth, cryst struct, uv, ir, tga*)

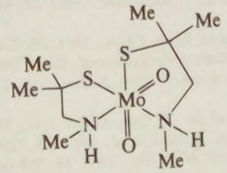
IC-007150

$C_{10}H_{24}MoN_2O_2S_2$

Bis[1,1-dimethyl-2-(*N*-methylamino)ethylthiolato]dioxomolybdenum(*VI*)

*Bis[2-methyl-1-(methylamino)-2-propanethiolato-*N,S] *dioxomolybdenum*(VI), *11CI, 10CI*

[74005-67-7]



M 364.3
Skew trapezoidal bipyramid (not octahedral). Synth. from $MoO_2(acac)_2$ + $MeNHCH_2C(CH_3)_2SH$. Yellow cryst. (MeOH). Soln. dec. after several days in air. Sol. MeOH, MeCN, $CHCl_3$.

Stiefel, E.I. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 3624 (*cryst struct, exafs*)
Corbin, J.L. *et al*, *Inorg. Chem.*, 1984, **23**, 3404 (*synth, ir, pmr*)
Berg, J.M. *et al*, *Inorg. Chem.*, 1984, **23**, 3412 (*cryst struct*)
Willis, L.J. *et al*, *Inorg. Chem.*, 1986, **25**, 4289 (*ir, raman*)

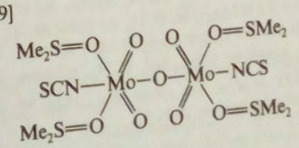
IC-007151

$C_{10}H_{24}Mo_2N_2O_9S_6$

Tetrakis(dimethyl sulfoxide)-μ-oxotetraoxobis(thiocyanato-*N*)dimolybdenum

μ-Oxobis[isothiocyanatobis[dimethylsulfoxide] dioxomolybdenum(VI)]. *μ-Oxotetraoxotetrakis[sulfinylbis[methane]-O]bis(thiocyanato-N)dimolybdenum, 11CI*

[86592-76-9]



M 700.5
Pale-yellow cryst.

Shibahara, T. *et al*, *Inorg. Chim. Acta*, 1983, **76**, L315 (*cryst struct, synth, ir*)

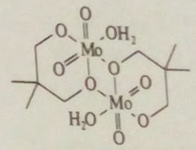
$C_{10}H_{24}Mo_2O_{10}$

Diaquabis[μ-(2,2-dimethyl-1,3-propanediolato(2−)-O^1:O^1,O^3)]tetraoxodimolybdenum(*VI*), 10CI

IC-007152

Bis-μ-(2,2-dimethylpropane-1,3-diolato) bis(aquodioxomolybdenum)(VI)

[61267-47-8]



M 496.1
Small pale brown translucent cryst.

Chew, C.K. *et al*, *J. Cryst. Mol. Struct.*, 1975, **5**, 413 (*cryst struct, synth*)
Knobler, C. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 248 (*ir, analogues*)

IC-007153

$C_{10}H_{24}N_2NiO_4S_6$

Tetrakis(dimethyl sulfoxide-*S*)bis(thiocyanato-*N*)nickel(*II*)

Tetrakis[sulfinylbis[methane]-S]bis(thiocyanato-N)nickel, 9CI. Bis(isothiocyanato)tetrakis(methylsulfoxide)nickel, 8CI

[32491-07-9]

$$Ni(NCS)_2[S(O)Me_2]_4$$

M 487.3
trans-Octahedral. Green solid.

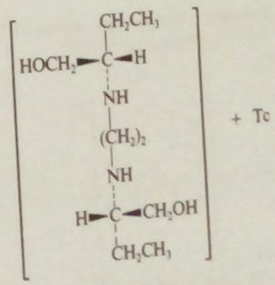
Cotton, F.A. *et al*, *J. Inorg. Nucl. Chem.*, 1961, **17**, 62 (*synth*)

IC-007154

$[C_{10}H_{24}N_2O_2Tc]$

2,2'-(1,2-Ethanediyldiimino)bis(1-butanol) technetium complex

N,N'-Di[(1-Hydroxymethyl)propyl]ethylenediamine technetium complex. Ethambutol-Tc. Technetium - ethambutol



S,S-form

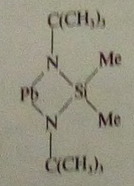
Deprotonated ligand probably bonded to $TcO^{3\oplus}$ core; chemically ill-characterised complex. Synth. by H_3PO_2 reduction of $TcO_4^{\ominus}$ + ligand. Combination of Tc with a potent tuberculostatic agent. Water-stable at physiol. pH.

Causse, J.E. *et al*, *Appl. Radiat. Isot.*, 1990, **41**, 493 (*synth, ms, chromatog, pharmacokinetics*)

$C_{10}H_{24}N_2PbSi$ IC-007155

[Dimethylsilylenebis(*tert*-butylimido-*N*,*N'*]lead

[84806-16-6]



M 407.5

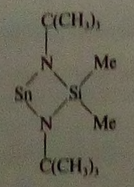
Synth. from $PbCl_2$ and $Me_2Si(N^tBuLi)_2$.

Veith, M. *et al*, *Z. Naturforsch., B*, 1982, **37**, 1375 (*synth*)
Veith, M. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 89 (*reactions*)

$C_{10}H_{24}N_2SiSn$ IC-007156

[Dimethylsilylenebis(*tert*-butylimido-*N*,*N'*)]tin

[54724-62-8]



M 319.1

Synth. from $Me_2Si(N^tBuLi)_2$ and $SnCl_2$. Red liq. Mp 5°. $Bp_{0.1}$ 55-57°.

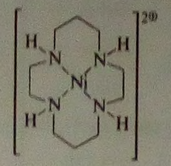
Veith, M. *et al*, *Angew. Chem., Int. Ed. Engl.*, 1975, **14**, 263 (*synth*)
Veith, M. *et al*, *Z. Naturforsch., B*, 1982, **37**, 1375; 1983, **38**, 1054 (*synth*)
Veith, M. *et al*, *Z. Anorg. Allg. Chem.*, 1984, **513**, 89 (*reactions*)
Veith, M. *et al*, *Chem. Ber.*, 1985, **118**, 1600 (*reactions*)
Veith, M. *et al*, *J. Organomet. Chem.*, 1985, **293**, 161 (*reactions*)

$C_{10}H_{24}N_4Ni^{2\oplus}$ IC-007157

(1,4,8,11-Tetraazacyclotetradecane)nickel(*II*)(2+), 9Cl

Cyclamnickel(2+). ([*14*]*AneN*$_4$)*nickel*(II)

[46365-93-9]



M 259.0 (ion)

Most commonly studied saturated macrocyclic tetramine complex. Work includes isomerism, oxidation, alkylation, catalytic conversion e.g. of CO_2 to CO. Salts are diamagnetic square planar. Complexes with additional coordinated ligands also known, e.g. Dichloro(1,4,8,11-tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})nickel(*II*), IC-007143 and Diaqua(1,4,8,11-tetraazacyclotetradecane)nickel(*II*)(2+), IC-007184.

Diperchlorate: [15220-72-1].
Golden-yellow cryst. Sol. H_2O, MeOH.
▷ Potentially explosive.

[52610-79-4, 57456-82-3]

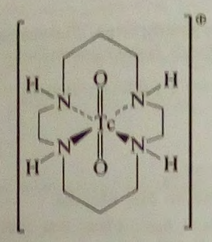
Beley, M. *et al*, *J. Am. Chem. Soc.*, 1986, **108**, 7461 (*catalysis*)
Compr. Coord. Chem., Pergamon, Oxford, 1987, **5**, 238 (*rev, bibl*)

$C_{10}H_{24}N_4O_3Tc^{\oplus}$ IC-007158

Dioxo(1,4,8,11-tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})technetium(*V*)(1+), 1Cl

Dioxo(*cyclam*)*technetium*(V)(*1+*)

[77136-42-6]



M 331.2 (ion)

trans-Octahedral cation. Synth. from $TcO_4^{\ominus}$ + cyclam by $S_2O_4^{2\ominus}$ reduction, or by ligand exchange from other complexes. Insufficiently lipophilic for diagnostic use.

Perchlorate: [77136-44-8].
Yellow-orange cryst. + H_2O. Sol. H_2O; insol. $CHCl_3$.
▷ Potentially explosive.

[78017-68-2]

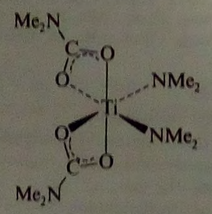
Troutner, D.E. *et al*, *J. Nucl. Med.*, 1980, **21**, 443 (*electrophoresis, biodistribn*)
Zuckman, S.A. *et al*, *Inorg. Chem.*, 1981, **20**, 2386 (*cryst struct*)
Simon, J. *et al*, *Radiochem. Radioanal. Lett.*, 1981, **47**, 111 (*synth*)
Volkert, W.A. *et al*, *Int. J. Appl. Radiat. Isot.*, 1982, **33**, 891 (*synth*)
Hoffman, T.J. *et al*, *Int. J. Appl. Radiat. Isot.*, 1984, **35**, 223 (*hplc*)
Hoffman, T.J. *et al*, *J. Nucl. Med.*, 1987, **28**, 729 (*analogues*)
Franz, J. *et al*, *Nucl. Med. Biol.*, 1987, **14**, 569 (*analogue*)

$C_{10}H_{24}N_4O_4Ti$ IC-007159

Bis(dimethylamido)bis(*N*,*N*-dimethylcarbamato)titanium(*IV*)

Bis(*dimethylcarbamato*-O,O')*bis*(N-*methylmethanaminato*)*titanium*(IV), *10Cl*

[62355-96-8]



M 312.2

Distorted octahedral with *cis*-N. Synth. by insertion of $2CO_2$ into $Ti(NMe_2)_4$ in C_6H_6 or toluene. If the amount of CO_2 is varied other compds. are formed. Red, moisture sensitive solid. Sol. C_6H_6, toluene, hexane.

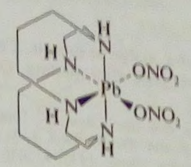
Chisholm, M.H. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 792 (*cryst struct, synth, mechanism, pmr, ir*)

$C_{10}H_{24}N_6O_6Pb$ IC-007160

Bis(nitrato-*O*)(1,4,8,11-tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})lead(*II*), 9Cl

(*1,4,8,11-Tetraazacyclotetradecane*)*lead*(II) *nitrate*

[69525-37-7]



M 531.5

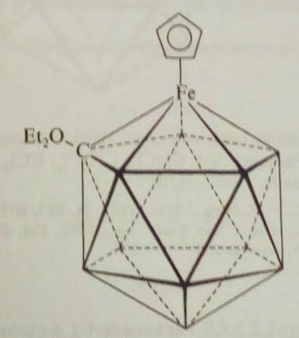
cis-Octahedral geometry. Prepd. by dissolving $Pb(NO_3)_2$ in dry DMSO and adding solid 1,4,8,11-tetraazacyclotetradecane. Cryst. (DMSO/MeOH).

Alcock, N.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1979, 1486 (*synth, cryst struct, nmr*)

$C_{10}H_{25}B_{10}FeO$ IC-007161

(η^5-2,4-Cyclopentadien-1-yl)[(7,8,9,10,11-η)-1,2,3,4,5,6,8,9,10,11-decahydro-7-[1,1-oxybis[ethane]]-7-carbaundecaborato(2−)]iron, 10Cl

[63090-63-1]



M 325.2

closo-. Dark green feathery cryst. (CH_2Cl_2/hexane). Sol. CH_2Cl_2.

Schultz, R.V. *et al*, *J. Organomet. Chem.*, 1977, **125**, 115 (*synth, cryst struct, ir, B-11 nmr, ms*)

$C_{10}H_{25}O_5Pa$ IC-007162

Protactinium(*V*) ethoxide

Protactinium pentaethoxide. *Pentaethoxyprotactinium*(V)

$Pa(OEt)_5$

M 456.3

Oligomeric in soln. (approx. hexamer). Yellow-white solid. Sol. C_6H_6. Bp > 300°.

Maddock, A.G. *et al*, *Radiochim. Acta*, 1972, **18**, 71 (*synth, ir*)
Bagnall, K.W. *et al*, *J. Chem. Soc., Dalton Trans.*, 1975, 1249 (*synth, use*)

$C_{10}H_{25}O_5U$ IC-007163

Uranium(*V*) ethoxide

Pentaethoxyuranium(V). *Uranium pentaethoxide*

[10405-34-2]

$U(OEt)_5$

M 463.3

V. air- and moisture-sensitive dark-brown liq. Sol. EtOH, Et_2O, C_6H_6, $CHCl_3$, CCl_4. d^{25} 1.711. Bp 150° *in vacuo*. Dist. <170° under reduced pressure.

Jones, R.G. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 4287 (*synth*)
Karraker, D.G., *Inorg. Chem.*, 1964, **3**, 1618 (*synth, uv*)
Karraker, D.G. *et al*, *J. Inorg. Nucl. Chem.*, 1969, **31**, 711 (*pmr, magnetism*)
Traverso, U. *et al*, *Inorg. Nucl. Chem. Lett.*, 1974, **10**, 771 (*synth, ir*)
Sostero, S. *et al*, *Inorg. Chim. Acta*, 1976, **19**, 229 (*synth, uv*)
Inorg. Synth., 1982, **21**, 165 (*synth*)
Eller, P.G. *et al*, *Inorg. Chem.*, 1983, **22**, 3184 (*pmr*)

$C_{10}H_{26}BN_3$ IC-007164

Bis(diethylamino)(dimethylamino)borane

N,N,N',N'-*Tetraethyl*-N'',N''-*dimethylboranetriamine*, *11Cl*. *Dimethylaminobis*(*diethylamino*)*borane*

[82821-76-9]

$(Et_2N)_2BNMe_2$

M 199.1

Sensitive to moisture. Sol. $CHCl_3$.

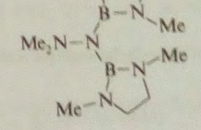
Govesnard, J.P., *Nouv. J. Chim.*, 1982, **6**, 143 (*nmr*)

$C_{10}H_{26}B_2N_6$ IC-007165

2,2'-(2,2-Dimethylhydrazono)bis[1,3-dimethyl-1,3,2-diazaborolidine], 10Cl

N,N-*Bis*-2-(*1,3-dimethyl-1,3,2-diazaboracyclopentyl*)-N',N'-*dimethylhydrazine*. N,N-*Bis*(*1,3-dimethyl-1,3,2-diazaborolan-2-yl*)-N',N'-*dimethylhydrazine*

[62567-26-4]



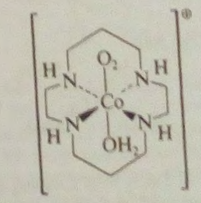
M 251.9

Oil, sensitive to moisture, relatively high thermal stability under inert atmosphere. Bp_1 81-82°.

Christmas, B.K. *et al*, *Z. Naturforsch., B*, 1977, **32**, 157 (*synth, ir, ms, nmr*)
Niedenzu, K. *et al*, *Z. Anorg. Allg. Chem.*, 1978, **439**, 103 (*synth*)

$C_{10}H_{26}CoN_4O_3^{\oplus}$ IC-007166

Aquaperoxy(1,4,8,11-tetraazacyclotetradecane)cobalt(*III*)(1+)



M 309.2 (ion)

Not isol. Formed on reduction of the corresp. superoxo complex.

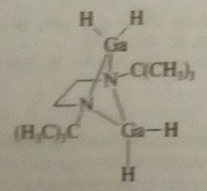
Kumar, K. *et al*, *Inorg. Chem.*, 1984, **23**, 2447 (*formn, kinetics*)

$C_{10}H_{26}Ga_2N_2$ IC-007167

[μ-[*N,N'*-Bis(1,1-dimethylethyl)-1,2-ethanediaminato(2−)-*N,N':N,N'*]]tetrahydrodigallium, 9CI

1,4-Di-tert-butyl-1,4-diaza-5,6-digallabicyclo[2.1.1]pentane. Tetrahydro[μ-[2,2,7,7-tetramethyl-3,6-diazaoctanato(2−)-N,N':N,N']]digallium

[130950-16-2]



M 313.7

Synth. from GaH_2NMe_2 and $^tBuN{=}C{-}C{=}N{-}^tBu$ in hexane. White air- and moisture-sensitive cryst. Mp 107° dec. Subl.$_{0.01}$ 95°. Ir ν_{Ga-H} 1920, 1870 cm^{-1}.

Henderson, M.J. *et al., J. Chem. Soc., Chem. Commun.*, 1990, 1203 (*synth, nmr, cmr, cryst struct*)

$C_{10}H_{27}ClCoOP_3$ IC-007168

Carbonylchlorotris(trimethylphosphine)cobalt, 9CI

[55449-08-6]

$(Me_3P)_3CoCl(CO)$

M 350.6

Air-sensitive wine-red cryst. (Et_2O). Spar. sol. pentane. Mp 94° dec. Ir ν_{CO} 1877 cm^{-1} (nujol).

Klein, H.-F. *et al., Inorg. Chem.*, 1975, **14**, 473 (*synth, ir, pmr*)

$C_{10}H_{27}CoIOP_3$ IC-007169

Carbonyliodotris(trimethylphosphine)cobalt, 9CI

[53432-14-7]

$(Me_3P)_3CoI(CO)$

M 442.0

Air-sensitive red cryst. (pentane or Et_2O). Spar. sol. Et_2O. Mp 130-132°. Ir ν_{CO} 1882 cm^{-1} (nujol). Dec. >170°.

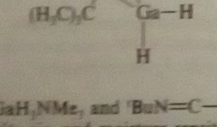
Klein, H.-F. *et al., Inorg. Chem.*, 1975, **14**, 473 (*synth, ir, pmr*)

$C_{10}H_{27}N_4Ta$ IC-007170

(*tert*-Butylimido)tris(dimethylamido)tantalum(*V*)

Tris(N-methylmethanaminato)[2-methyl-2-propanaminato(2−)]tantalum(V), *10CI*

[69039-11-8]



M 384.2

Synth. by reaction of $TaCl_5$ with $LiNMe_2$ and lithium *tert*-butylamide. White solid. Sol. C_6H_6. Mp 68-69°.

Nugent, W.H. *et al., J. Chem. Soc., Chem. Commun.*, 1978, 579 (*synth, cryst struct, pmr*)

$C_{10}H_{27}NiOP_3$ IC-007171

Carbonyltris(trimethylphosphine)nickel, 9CI, 8CI

Tris(trimethylphosphine)carbonylnickel

[15376-84-8]

$Ni(CO)(PMe_3)_3$ (C_{3v})

M 314.9

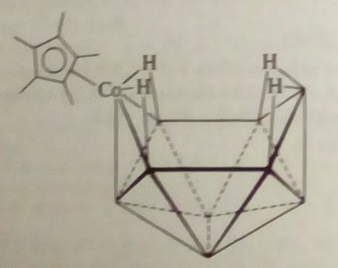
White gummy solid, stable in dry air. Compound solidifies to a transparent glass after melting. Dec. begins at 120°/0.01 mm.

Bignorgne, M. *et al., Bull. Soc. Chim. Fr.*, 1960, 1986 (*synth, ir*)
Bouquet, G. *et al., J. Mol. Struct.*, 1968, **1**, 211 (*ir, raman*)
Matheu, R. *et al., Inorg. Chem.*, 1970, **9**, 2030 (*nmr*)

$C_{10}H_{28}B_9Co$ IC-007172

[(1,2,3,4,5-η)-1,2,3,4,5-Pentamethyl-2,4-cyclopentadien-1-yl][tridecahydrononaborato(1−)]cobalt, 10CI

[80145-59-1]



M 304.5

nido-. Air-stable burgundy cryst. (by chromatog. with CH_2Cl_2/hexane). Sol. $CHCl_3$, CH_2Cl_2, CCl_4. Diamagnetic. Dec. at 250°.

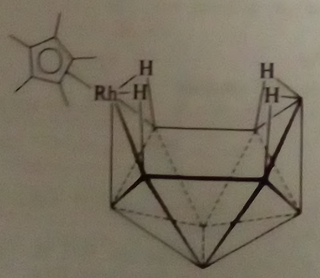
Venable, T.L. *et al., Inorg. Chem.*, 1982, **21**, 887, 895 (*B-11 nmr*)
Venable, T.L. *et al., J. Am. Chem. Soc.*, 1982, **104**, 4716 (*synth, pmr, ms, ir, cryst struct*)

$C_{10}H_{28}B_9Rh$ IC-007173

[(1,2,3,4,5-η)-1,2,3,4,5-Pentamethyl-2,4-cyclopentadien-1-yl][(6,7,8-η)-tridecahydrononaborato(2−)-*H*^{6},*H*^{7},*H*^{8}]rhodium, 11CI

6-(η^5-Pentamethylcyclopentadienyl)-6-rhodadecaborane

[104601-71-0]



M 348.5

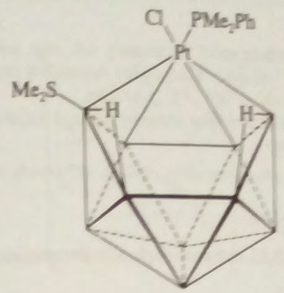
nido-. Air-stable orange-red cryst. (CH_2Cl_2/pet. ether). Sol. CH_2Cl_2.

Fontaine, X.L.R. *et al., J. Chem. Soc., Dalton Trans.*, 1986, 547 (*synth, pmr, B-11 nmr, cryst struct*)

$C_{10}H_{29}B_{10}ClPPtS$ IC-007174

Chloro(dimethylphenylphosphine)[(6,7,8,9-η)-undecahydro-6-[thiobis[methane]]decaborato(1−)]platinum, 11CI

[96120-49-9]



M 550.0

nido-struct. proposed on basis of ^{11}B nmr. Synth. from $PtCl_2(PMe_2Ph)_2$ and $(Me_2S)_2B_{10}H_{12}$ in CH_2Cl_2.

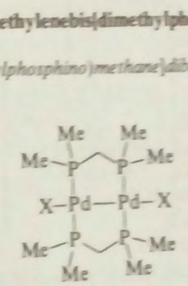
Greenwood, N.N. *et al., J. Chem. Soc., Dalton Trans.*, 1984, 2487 (*B-11 nmr, P-31 nmr*)

$C_{10}H_{28}Br_2P_4Pd_2$ IC-007175

Dibromobis-μ-[methylenebis[dimethylphosphine]-*P,P'*]dipalladium

Bis-μ-[bis(dimethylphosphino)methane]dibromodipalladium

[98088-57-4]



X=Br

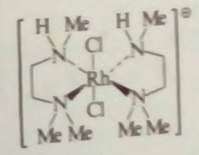
M 644.8

Orange cryst. (CH_2Cl_2/Et_2O). Sl. sol. aq. solns. Ir ν_{Pd-Br} 175 cm^{-1}; Raman ν_{Pd-Br} 169, ν_{Pd-Pd} 123 cm^{-1}.

Kullberg, M.L. *et al., Inorg. Chem.*, 1985, **24**, 3589 (*synth, ir, raman, pmr, cmr, P-31 nmr, struct, str*)

$C_{10}H_{28}Cl_2N_4Rh^{\oplus}$ IC-007176

Dichlorobis(*N,N,N'*-trimethylethylenediamine)rhodium(*III*)(1+)



M 378.1 (ion)

Iodide: Yellow-orange solid.

Watt, G.W. *et al., J. Am. Chem. Soc.*, 1967, **89**, 1814 (*synth, ir, str*)

$C_{10}H_{28}Cl_2P_4Pd_2$ IC-007177

Dichlorobis-μ-[methylenebis[dimethylphosphine]-*P,P'*]dipalladium

Bis-μ-[bis(dimethylphosphino)methane]dichlorodipalladium

[89178-59-6]

As Dibromobis-μ-[methylenebis[dimethylphosphine]-*P,P'*] dipalladium, IC-007175 with

X = Cl

M 555.9

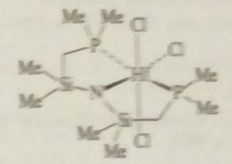
Catalyses watergas shift reaction. Yellow-orange cryst. (CH_2Cl_2/Et_2O). Sol. aq. solns., org. solvs. Ir ν_{Pd-Cl} 260 cm^{-1}; Raman ν_{Pd-Cl} 257, ν_{Pd-Pd} 140 cm^{-1}.

Kullberg, M.L. *et al., J. Mol. Chem.*, 1984, **1**, 171 (*str*)
Kullberg, M.L. *et al., Organometallics*, 1984, **3**, 632 (*synth, str*)
Kullberg, M.L. *et al., Inorg. Chem.*, 1985, **24**, 3589; 1986, **25**, 26 (*synth, ir, raman, pmr, cmr, str, P-31 nmr*)

$C_{10}H_{28}Cl_2HfNP_2Si_2$ IC-007178

[Bis[(dimethylphosphinomethyl)dimethylsilyl]amido-*N,P,P'*]trichlorohafnium(*IV*)

Trichloro[1-[(dimethylphosphino)methyl]-N-[[(dimethylphosphino)methyl]dimethylsilyl]-1,1-dimethylsilanaminato-N,P,P']hafnium(IV), *10CI*



M 565.3

Octahedral, only the *mer*-form exists in soln. based on pmr and cmr data.

***mer*-form** [94481-25-1]

Synth. from $HfCl_4$ and the Li salt of the ligand in toluene. Colourless solid. Sol. C_6H_6, CH_2Cl_2.

[94372-14-2]

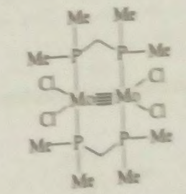
Fryzuk, M.D. *et al., Inorg. Chem.*, 1985, **24**, 642 (*synth, pmr, P-31 nmr, cryst struct*)

$C_{10}H_{28}Cl_4Mo_2P_4$ IC-007179

Tetrachlorobis[μ-[methylenebis[dimethylphosphine]-*P,P'*]]dimolybdenum(*II*), 11CI

Bis[μ-bis(dimethylphosphino)methane-P,P']dichlorotetrachlorodimolybdenum(II)

[104092-00-4]



M 605.9

Quadruply bonded: Mo—Mo 213.4, Mo—Cl 247.7, Mo—P 247.7 pm. Synth. from (a) $Mo_2(OAc)_4$ and dmpm in toluene, or (b) $K_4Mo_2Cl_8$ and dmpm in toluene/MeOH. Hygroscopic blue tetragonal cryst. (CH_2Cl_2/hexane) or monoclinic cryst. V. air- and moisture-sensitive in soln. Mod. sol. CH_2Cl_2, insol. hexane; sl. sol. MeCN, THF.

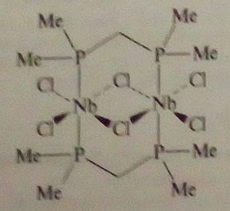
Cotton, F.A. *et al., Inorg. Chem.*, 1988, **25**, 3949 (*cryst struct, synths, ir, pmr, P-31 nmr, electrochem*)

$C_{10}H_{28}Cl_6Nb_2P_4$ IC-007180

Di-μ-chlorotetrachlorobis[μ-methylenebis[dimethylphosphine]-*P*,*P*']diniobium(*III*), 11Cl

Bis[bis(dimethylphosphino)methane]di-μ-chlorotetrachlorodiniobium(III)

[98858-57-2]



M 670.7

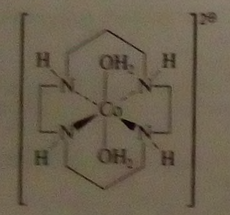
Synth. by adding a hexane soln. of the phosphine to $Nb_2Cl_4(THF)_2$ in toluene. Red cryst.

Cotton, F.A. *et al*, *Inorg. Chem.*, 1985, **24**, 4389 (*synth, cryst struct, ms*)

$C_{10}H_{29}CoN_4O_2^{2\oplus}$ IC-007181

Diaqua(1,4,8,11-tetraazacyclotetradecane-N^1,N^4,N^8,N^{11})cobalt(*II*)(2+), 10Cl

[46750-09-8]



M 295.2 (ion)

Approx. *trans*-octahedral cation. Oxygen uptake kinetics for this complex have been studied in aq. soln.

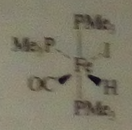
Diperchlorate: [65554-14-5].
Brown cryst. Sol. H_2O.
▷ Potentially explosive.

Chap, Y.M. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 123 (*synth, ur*)
Lai Wong, C. *et al*, *J. Am. Chem. Soc.*, 1980, **102**, 5511 (*kinetics*)

$C_{10}H_{29}FeIOP_3$ IC-007182

Carbonylhydroiodotris(trimethylphosphine)iron, 9Cl

[60753-48-4]



M 440.0

Light-brown cryst. (hexane).

Pankowski, M. *et al*, *J. Organomet. Chem.*, 1975, **97**, 105 (*synth, ir, pmr*)

$C_{10}H_{28}IrOP_3$ IC-007183

Carbonylhydrotris(trimethylphosphine)iridium, 11Cl

Hydridocarbonyltris(trimethylphosphine)iridium

[79568-60-8]

$IrH(CO)(PMe_3)_3$

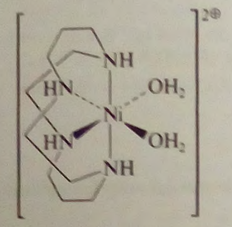
M 449.4

Sticky, off-white solid. Extremely sol. org. solvs. Ir 2010, 1900 cm^{-1} (nujol). Undergoes reversible protonation with HX (X = BF_4,PF_6) to give Carbonyldihydrotris(trimethylphosphine)iridium(1+), IC-007190.

Thorn, D.L., *Organometallics*, 1982, **1**, 197 (*synth, ir, pmr, props*)

$C_{10}H_{28}N_4NiO_2^{2\oplus}$ IC-007184

Diaqua(1,4,8,11-tetraazacyclotetradecane)nickel(*II*)(2+), 9Cl



cis-form

M 295.0 (ion)

Blue-violet solns.

cis-form [64616-26-8]

Chloride, dihydrate: [104194-92-5].
$C_{10}H_{32}Cl_2N_4NiO_4$ M 401.9
Mauve cryst. Sol. H_2O.

trans-form [78684-35-2]

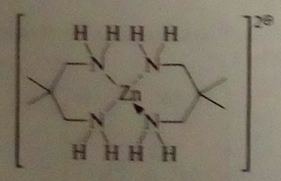
Detected only in soln.

[104485-30-5]

Herron, N. *et al*, *Inorg. Chim. Acta*, 1979, **36**, 89.
Billo, E.J., *Inorg. Chem.*, 1981, **20**, 4019.
Barefield, E.K. *et al*, *Inorg. Chem.*, 1986, **25**, 4197 (*synth, cryst struct*)

$C_{10}H_{28}N_4Zn^{2\oplus}$ IC-007185

Bis(2,2-dimethylpropane-1,3-diamine-*N*,*N*')zinc(2+), 12Cl



M 269.7 (ion)

Tetrahedral zinc.

Dichloride: [122627-38-7].
Cryst.

Diiodide: [122651-29-0].
$C_{10}H_{28}I_2N_4Zn$ M 523.5
Cryst. (MeOH).

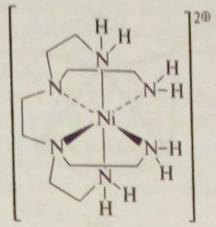
Massiocchi, N. *et al*, *Inorg. Chim. Acta*, 1989, **159**, 173 (*synth, cryst struct, ir, raman*)

$C_{10}H_{28}N_6Ni^{2\oplus}$ IC-007186

[4,7-Bis(2-aminoethyl)triethylenetetramine]nickel(2+), 8Cl

[N,N,N',N'-*Tetrakis*(2-*aminoethyl*)-1,2-*ethanediamine*]*nickel*(2+), *11Cl*. [N,N,N',N'-*Tetrakis*(2-*aminoethyl*)*ethylenediamine*]*nickel*(II)(2+). (*Penten*)*nickel*(2+)

[31252-70-7]



M 291.0 (ion)

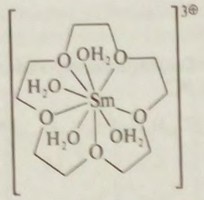
Strong complex in soln. (Log K = 19.3) but no salts isol.

Paoletti, P. *et al*, *Helv. Chim. Acta*, 1971, **54**, 243.

$C_{10}H_{28}O_9Sm^{3\oplus}$ IC-007187

Tetraaqua(15-crown-5)samarium(*III*)(3+)

Tetraaqua(1,4,7,10,13-*pentaoxacyclopentadecane*-O^1,O^4,O^7,O^{10},O^{13})*samarium*(3+), *11Cl*



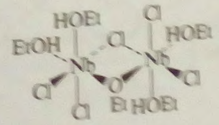
M 442.6 (ion)

Triperchlorate: [87651-92-1]. *Samarium*(III) *perchlorate 15-crown-5*
Plate-like cryst. + H_2O + 15-crown-5. Sol. MeCN. 9-Coordinate; contains one molecule of 15-crown-5 of crystallisation.
▷ Potentially explosive.

Lee, T.J. *et al*, *Acta Crystallogr., Sect. C*, 1983, **39**, 1357 (*cryst struct, synth*)

$C_{10}H_{29}Cl_2Nb_2O_5$ IC-007188

μ-Chlorotetrachloro-μ-ethoxytetrakis(ethanol)diniobium(*III*)



M 592.4

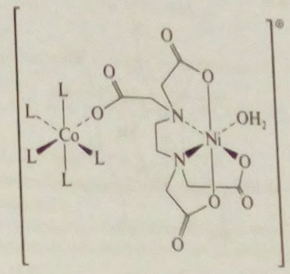
Bi-octahedral by analogy with the isopropyl compd. Synth. by reaction of Nb_2Cl_4(tetrahydrothiophene)$_3$ with EtOH in toluene. Brown solid.

Cotton, F.A. *et al*, *Inorg. Chem.*, 1985, **24**, 3509 (*synth, cryst struct*)

$C_{10}H_{29}CoN_7NiO_9^{\oplus}$ IC-007189

[Pentaamminecobalt(*III*)]-μ-(ethylenediaminetetraacetato)(aqua)nickel(*II*)(1+)

Pentaammine[*aquanickel*(II)][μ-[[1,2-*ethanediylbis*[N-(*carboxymethyl*)*glycinato*]](4−)-N,N',O,O',O^N:$O^{N'}$]]*cobalt*(III)(1+), *10Cl*



L = NH_3

M 509.0 (ion)

EDTA pentadentate to Ni, monodentate to Co. Also known for other metals replacing Ni.

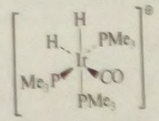
Perchlorate: [61916-05-0].
Solid +2H_2O. Sol. H_2O.
▷ Potentially explosive.

Ogino, H. *et al*, *Inorg. Chem.*, 1977, **16**, 1215 (*synth, ur*)

$C_{10}H_{29}IrOP_3^{\oplus}$ IC-007190

Carbonyldihydrotris(trimethylphosphine)iridium(1+), 11Cl

Dihydridocarbonyltris(trimethylphosphine)iridium(1+)



M 450.4 (ion)

mer-form

Undergoes reversible deprotonation with base (e.g. KO^{t}Bu) to give Carbonylhydrotris(trimethylphosphine)iridium, IC-007183.

Tetrafluoroborate: [79568-62-0].
White air-stable solid. Spar. sol. THF. Mp 132-136°. Ir 2095, 2040, 1998 cm^{-1} (nujol).

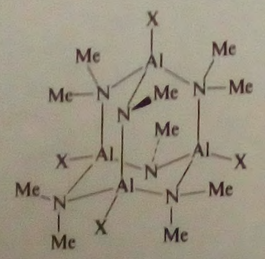
Thorn, D.L., *Organometallics*, 1982, **1**, 197 (*synth, ir, pmr, props*)

$C_{10}H_{30}Al_4Cl_4N_6$ IC-007191

Tetrachlorotetrakis(dimethylamino)bis(methylimino) tetraaluminium

Tetrachlorobis[μ-[methanaminato(2−)]]tetrakis[μ-(N-methylmethanaminato)]tetraaluminium, 9CI

[20982-79-0]



X = Cl

M 484.1

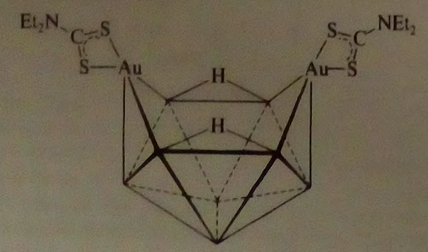
From $B_2(NMe_2)_4$ and $ClAl(NMe_2)_2$. Colourless cryst. Dissolves slowly in dil. acids. Sol. C_6H_6, CCl_4, $CHCl_3$, Et_2O; insol. hexane. Mp > 340°. Subl. $_{0.001}$ 220°.

Nöth, H. *et al, Chem. Ber.*, 1968, **101**, 3423 (*synth, ms*)
Thewalt, U. *et al, Chem. Ber.*, 1970, **103**, 2754 (*cryst struct*)
Nöth, H. *et al, Z. Naturforsch., B*, 1976, **31**, 1447 (*pmr, N-14 nmr, Al-27 nmr, reactions*)

$C_{10}H_{30}Au_2B_8N_2S_4$ IC-007192

[μ-[(3,4,5-η:6,7,8-η)-Decahydrooctaborato(2−)]] bis(diethylcarbamodithioato-*S,S'*)digold, 11CI

[92627-82-2]



M 787.0

arachno-. Bright-yellow cryst. (CH_2Cl_2/pet. ether by chromatog.). Sol. CH_2Cl_2, $CHCl_3$, C_6H_6.

Beckett, M.A. *et al, J. Chem. Soc., Dalton Trans.*, 1984, 1427 (*synth, cryst struct, pmr, B-11 nmr*)

$C_{10}H_{30}B_2N_2Si_2$ IC-007193

1,2-Bis(dimethylamino)-1,2-bis(trimethylsilyl)diborane(4)

N,N,N',N'-Tetramethyl-1,2-bis(trimethylsilyl)-1,2-diborane(4)diamine, 10CI

[64448-58-4]

$$Me_2NB(SiMe_3)—B(SiMe_3)NMe_2$$

M 256.1

No phys. props. reported, but presumably sensitive to air and moisture.

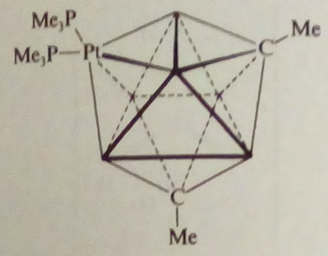
Fussstetter, H. *et al, Chem. Ber.*, 1977, **110**, 3172 (*nmr*)
Biffar, W. *et al, Chem. Ber.*, 1981, **114**, 49 (*nmr*)

$C_{10}H_{30}B_6P_2Pt$ IC-007194

[(4,5,7,8-η)-1,6-Dimethyl-1,6-dicarbaoctaborane(8)] bis(trimethylphosphine)platinum, 10CI

7,8-Dimethyl-9-bis(trimethylphosphine)-7,8-dicarba-9-platina-closo-nonaborane(8). 6,8-Dimethyl-1,1-bis(trimethylphosphine)-6,8-dicarba-1-platinaoctaborane

[55888-13-6]



M 472.2

closo-. Synth. from Pt (*trans*-stilbene) $(PMe_3)_2$ and *closo*-1,7-Me_2-1,7-C_2B_6H as major product. Yellow cryst. (Et_2O). Mp 173°.

Green, M. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 794 (*synth, cryst struct*)
Welch, A.J., *J. Chem. Soc., Dalton Trans.*, 1976, 225 (*cryst struct*)
Stone, F.G.A. *et al, J. Chem. Soc., Dalton Trans.*, 1979, 1679 (*synth, pmr, B-11, P-31, P-195 nmr, ir*)

$C_{10}H_{30}B_{20}N_2Pd_2^{2\ominus}$ IC-007195

(1,10-Phenanthroline)bis[undecahydrodecaborato(3−)] dipalladate(2−), 9CI

$$[(C_{10}H_8N_2)Pd_2(B_{10}H_{11})_2]^{2\ominus}$$

M 607.4 (ion)

Struct. unknown.

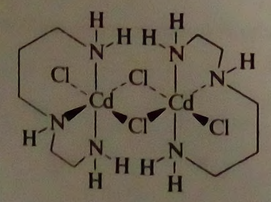
Bis-Et_4N salt: [60349-64-6].
Air-sensitive red needles (MeCN/2-butanone). Sol. MeCN.

Siedle, A.R. *et al, Inorg. Chem.*, 1976, **15**, 2838 (*synth, pmr, B-11 nmr, ir, uv-vis*)

$C_{10}H_{30}Cd_2Cl_4N_6$ IC-007196

Bis[(2-aminoethyl)-1,3-propanediamine-*N,N',N''*]di-μ-chlorodichlorodicadmium, 10CI

[75847-03-9]



M 601.0

Cryst. (aq. MeOH).

Monomer: [*2-Aminoethyl(3-aminopropyl)amine*]*cadmium dichloride*
$C_5H_{15}CdCl_2N_3$ M 300.5
Not separately obt.

Cannas, M. *et al, J. Chem. Soc., Dalton Trans.*, 1980, 2090 (*synth, cryst struct, pmr*)

$C_{10}H_{30}ClFeO_5S_5^{2\oplus}$ IC-007197

Chloropentakis(dimethyl sulfoxide-*O*)iron(*III*)(2+)

Chloropentakis[sulfinylbis[methane]-O]iron(2+), 11CI

$$[FeCl(O{=}SMe_2)_5]^{2\oplus}$$

M 481.9 (ion)

Octahedral cation.

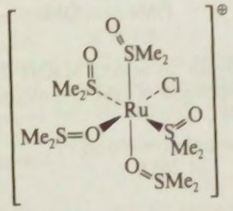
Hexachloro-μ-oxodiferrate(2−): [66574-24-1].
Chloropentakis(dimethyl sulfoxide-O)iron(2+) μ-oxobis[trichloroferrate(1−)]
$C_{10}H_{30}Cl_7Fe_3O_6S_5$ M 822.3
Synth. e.g. from Fe + a 1:1:2 mix DMSO: CCl_4: C_6H_6 heated at 120°; residue dissolved in EtOH and heated at 50°. Red-brown cryst. Mp 144°.
Bis[tetrachloroferrate(1−)]: [66609-86-7].
Forms in same synth. as hexachloro-μ-oxoferrate salt. Yellow cryst. Subl.$_{0.1}$ 210°.

Arutyanyan, L.D. *et al, Koord. Khim.*, 1978, **4**, 441 (*struct*)
Lavrent'ev, I.P. *et al, Koord. Khim.*, 1979, **5**, 1484 (*synth, mössbauer, struct*)
Lavrent'ev, I.P. *et al, Transition Met. Chem.*, 1980, **5**, 193 (*synth, struct, mössbauer*)
Gusakovskaya, I.G. *et al, Zh. Strukt. Khim.*, 1982, **23**, 53 (*mössbauer, phases*)
Ponomarev, V.I. *et al, Kristallografiya*, 1984, **29**, 910 (*cryst struct*)

$C_{10}H_{30}ClO_5RuS_5^{\oplus}$ IC-007198

Chloropentakis(dimethyl sulfoxide)ruthenium(*II*)(1+)

Chlorobis[sulfinylbis[methane]-O]tris[sulfinylbis[methane]-S] ruthenium(1+), 10CI



M 527.1 (ion)

mer, cis -Config. of 3 S-bonded and 2 O-bonded DMSO ligands. Prep. by treating Dichlorotetrakis(dimethyl sulfoxide)ruthenium(*II*), IC-006280 with $AgBF_4$ in DMSO. Sol. DMSO, H_2O.

Tetrafluoroborate: [72907-39-2].
Yellow solid. Ir ν_{RuCl} 246 cm^{-1}.

Barnes, J.R. *et al, J. Chem. Res. (S)*, 1979, 350; *J. Chem. Res. (M)*, 1979, 4301 (*synth, pmr, ir*)

$C_{10}H_{30}Cl_3O_5S_5U^{\oplus}$ IC-007199

Trichloropentakis(dimethyl sulfoxide)uranium(*IV*)(1+)

Trichloropentakis[sulfinylbis[methane]]uranium(IV)(1+)

$$[UCl_3(O{=}SMe_2)_5]^{\oplus}$$

M 735.0 (ion)

Chloride: see *Tetrachloropentakis(dimethyl sulfoxide) uranium*(IV), *IC-007203*
Perchlorate: Green cryst. ($MeNO_2$/EtOAc).
▷ Potentially explosive.

du Preez, J.G.H. *et al, J. Inorg. Nucl. Chem.*, 1974, **36**, 1795 (*synth, props*)

$C_{10}H_{30}Cl_4O_5PaS_5$ IC-007200

Tetrachloropentakis(dimethyl sulfoxide)protactinium(*IV*)

Tetrachloropentakis[sulfinylbis[methane]]protactinium(IV). *Protactinium*(IV) *chloride pentakis(dimethyl sulfoxide)*

[19403-39-5]

$$PaCl_4(O{=}SMe_2)_5$$

M 763.5

Bright yellow solid. Oxidizes on keeping in dry Ar over 1-2 days.

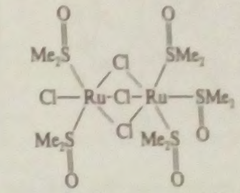
Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 465 (*synth, ir*)

$C_{10}H_{30}Cl_4O_5Ru_2S_5$ IC-007201

Tri-μ-chlorochloropentakis(dimethyl sulfoxide-*S*) diruthenium(*II*)

Tri-μ-chlorochloropentakis[sulfinylbis[methane]-S] diruthenium. Ruthenium(II) *chloride 2.5 dimethyl sufoxide*

[69501-71-9]



M 734.6

Approx. bioctahedral. Prepd. by heating a wet toluene soln. of Dichlorotetrakis(dimethyl sulfoxide) ruthenium(*II*), IC-006280 under reflux. Orange cryst. Sol. CH_2Cl_2. Mp 250° dec. Ir ν_{SO} 1135, 1115, 1095 cm^{-1}.

Heath, G.A. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 2429 (*synth, ir, cmr, pmr, electrochem*)

$C_{10}H_{30}Cl_4O_5S_5Th$ IC-007202

Tetrachloropentakis(dimethyl sulfoxide)thorium(*IV*)

Tetrachloropentakis[sulfinylbis(methane)-O]thorium(IV)

$$ThCl_4(O{=}SMe_2)_5$$

M 764.5

Believed to be ionic in solid state and polar solvs. Does not lose DMSO *in vacuo*, but on treatment with hot Me_2CO affords Tetrachlorotris(dimethyl sulfoxide) thorium(*IV*), IC-005354.

Solid state-form
Trichloropentakis(dimethyl sulfoxide)thorium(IV) *chloride.*
Trichloropentakis[sulfinylbis[methane]]thorium(1+) chloride
White cryst. Sol. $MeNO_2$, MeCN.

Bagnall, K.W. *et al, J. Chem. Soc. A*, 1968, 465 (*synth, ir*)
Alvey, P.J. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 2308

$C_{10}H_{30}Cl_4O_5S_5U$ IC-007203

Tetrachloropentakis(dimethyl sulfoxide)uranium(*IV*)

Tetrachloropentakis[sulfinylbis[methane]-O]uranium(IV), *9CI*

[40827-59-6]

$$UCl_4(O{=}SMe_2)_5$$

M 770.5

Probably ionic in solid state and in polar solvs.

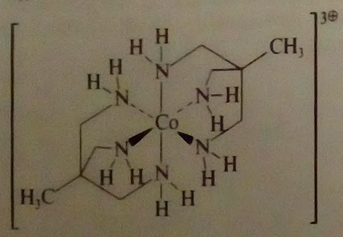
Solid state-form

Trichloropentakis(dimethyl sulfoxide)uranium(IV) *chloride. Trichloropentakis[sulfinylbis[methane]] uranium*(1+) *chloride*
Green cryst. Sol. $MeNO_2$. See also Trichloropentakis(dimethyl sulfoxide)uranium(*IV*)(1+), IC-007199.

Bagnall, K.W. *et al*, *J. Chem. Soc. A*, 1968, 465 (*synth, ir*)
du Preez, J.G.H. *et al*, *Inorg. Nucl. Chem. Lett.*, 1973, **9**, 99 (*synth*)
du Preez, J.G.H. *et al*, *J. Inorg. Nucl. Chem.*, 1974, **36**, 1795 (*synth*)
Sakurai, H. *et al*, *J. Inorg. Nucl. Chem.*, 1980, **42**, 66 (*magnetism, ir*)

$C_{10}H_{30}CoN_6^{3\oplus}$ IC-007204

Bis[1,1,1-tris(aminomethyl)ethane]cobalt(*III*)(3+)
Bis[2-(aminomethyl)-2-methyl-1,3-propanediamine-N,N′,N″] *cobalt*(3+), *11CI, 10CI*



M 293.3 (ion)
In soln., cation has interconvertible meso and racemic conformations. Racemic conformer has been resolved in solid state.

(±)-form

Trichloride: [60909-16-2].
Bright orange hexagonal platelets + $1H_2O$. Sol. H_2O.
Dichloride, perchlorate: [73953-33-0].
Yellow cryst. (aq. HCl).

[60934-82-9, 60934-83-0]

Geue, R.J. *et al*, *Inorg. Chem.*, 1977, **16**, 231 (*cryst struct, conformn, abs config, cd, pmr*)
Flückiger, J.R. *et al*, *Inorg. Chem.*, 1980, **19**, 2493 (*synth, pmr, uv-vis*)

$C_{10}H_{30}F_{10}N_5P_5Ru$ IC-007205

Pentakis[(dimethylamino)difluorophosphine]ruthenium(0)
Pentakis(dimethylphosphoramidous difluoride-P)*ruthenium*
[68010-21-9]

$Ru(PF_2NMe_2)_5$

M 666.3
Trigonal bipyramidal. Fluxional in soln. Synth. by the reductive elimination of HOAc from $Ru(PPh_3)_3H(OAc)$ in the presence of an excess of PF_2NMe_2. White solid. Sol. $CHCl_3$, CH_2Cl_2.

Al-Ohaly, A.-R. *et al*, *J. Organomet. Chem.*, 1981, **205**, 99 (*synth, nmr, ms*)

$C_{10}H_{30}N_5Nb$ IC-007206

Pentakis(dimethylamido)niobium(*V*)
Pentakis(dimethylamino)niobium(V). *Niobium*(V) *dimethylamide*

$Nb(NMe_2)_5$

M 313.2
Square pyramidal. Synth. by adding $NbCl_5$ to a suspension of $LiNMe_2$ in pentane. Brown solid. $Subl._{0.1}$ 100°. The same reaction with other $LiNR_2$ (R ≠ Me) leads mainly to reduction to Nb(*IV*).

Bradley, D.C. *et al*, *Can. J. Chem.*, 1962, **40**, 449 (*synth*)

$C_{10}H_{30}N_5Ta$ IC-007207

Pentakis(dimethylamido)tantalum(*V*)
Pentakis(dimethylamino)tantalum(V). *Tantalum*(V) *dimethylamide*

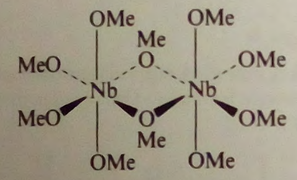
$Ta(NMe_2)_5$

M 401.3
Synth. by adding $TaCl_5$ to a suspension of $LiNMe_2$ in pentane. Pale yellow solid. $Subl._{0.1}$ 100°. Other $Ta(NR_2)_5$ species may be isolated similarly (R = Et, Pr, Bu).

Bradley, D.C. *et al*, *Proc. Chem. Soc., London*, 1959, 225 (*synth*)
Bradley, D.C. *et al*, *Can. J. Chem.*, 1962, **40**, 1355 (*synth*)

$C_{10}H_{30}Nb_2O_{10}$ IC-007208

Di-μ-methoxyoctamethoxydiniobium(*V*), 11CI
Diniobium(V) *decamethoxide. Niobium*(V) *methoxide dimer*
[18533-43-2]



M 496.1
Bi-octahedral. Synth. by adding MeOH then excess NH_3 to a C_6H_6 suspension of $NbCl_5$. Colourless solid. Mp 60°. $Bp_{0.05}$ 156°.

Monomer: Pentamethoxyniobium(V)
$C_5H_{15}NbO_5$ M 248.0
Unknown.

Bradley, D.C. *et al*, *J. Chem. Soc.*, 1956, 2381 (*synth*)
Bradley, D.C. *et al*, *J. Chem. Soc. A*, 1968, 219 (*nmr studies of ligand exch*)
Reiss, J.G. *et al*, *Chimia*, 1976, **30**, 481 (*cryst struct, nmr*)
Pinkerton, A.A. *et al*, *Inorg. Chem.*, 1976, **15**, 1196 (*cryst struct*)

$C_{10}H_{30}O_2P_4Pd_2$ IC-007209

Dihydroxybis-μ-[methylenebis[dimethylphosphine]-*P,P′*] dipalladium
Bis-μ-[bis(dimethylphosphino)methane]dihydroxydipalladium
[89178-61-0]

As Dibromobis-μ-[methylenebis[dimethylphosphine]-*P:P′*] dipalladium, IC-007175 with

X = OH

M 519.0
Not isol. Obt. in aq. soln. Solns. are orange. Raman $\nu_{Pd\text{-}OH}$ 351, $\nu_{Pd\text{-}Pd}$ 140 cm^{-1}.

Kullberg, M.L. *et al*, *Organometallics*, 1984, **3**, 632 (*synth, props*)
Kullberg, M.L. *et al*, *Inorg. Chem.*, 1985, **24**, 3589 (*synth, raman, pmr, P-31 nmr, uv*)

$C_{10}H_{30}O_6S_5V^{2\oplus}$ IC-007210

Pentakis(dimethyl sulfoxide)oxovanadium(*IV*)(2+)
Oxopentakis(dimethyl sulfoxide)vanadium(IV)(2+).
Oxopentakis[sulfinylbis[methane]-O]*vanadium*(2+) *11CI*

$[VO(O{=}SMe_2)_5]^{2\oplus}$ (C_{4v})

M 457.6 (ion)
Octahedral.
Dibromide: [52646-81-8].
Synth. by adding $VOBr_3$ to a soln. of DMSO in cyclohexane. Pale green solid.
Diiodide: [18582-11-1].
Synth. from $VOSO_4$ and BaI_2 and dissolving the product in excess DMSO. Blue solid.
Diperchlorate: [19325-19-0].
Synth. from $VO(ClO_4)_2$ and excess DMSO.
▷ Potentially explosive.

Nicholls, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 2751 (*synth, ir, bromide*)
Khodashova, T.S. *et al*, *Koord. Khim.*, 1978, **4**, 1909; *CA*, **90**, 64989v (*cryst struct, perchlorate*)
Collison, D. *et al*, *J. Chem. Soc., Dalton Trans.*, 1980, 667 (*uv-vis*)
Seifert, H.J. *et al*, *Z. Anorg. Allg. Chem.*, 1981, **479**, 32 (*synth, cryst struct, iodide*)
Harada, M. *et al*, *Chem. Lett.*, 1984, 1195 (*synth, perchlorate*)
Kaya, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 2648 (*props*)

$C_{10}H_{30}O_7S_5U^{2\oplus}$ IC-007211

Pentakis(dimethyl sulfoxide)dioxouranium(*VI*)(2+)
Dioxopentakis[sulfinylbis[methane]-O]*uranium*(VI)(2+)

$[UO_2(O{=}SMe_2)_5]^{2\oplus}$

M 660.7 (ion)
Main $UO_2^{2\oplus}$ sp. in Me_2CO/DMSO solns. as shown by nmr. Similar ions formed with H_2O, urea, pyridine-*N*-oxide, DMF.

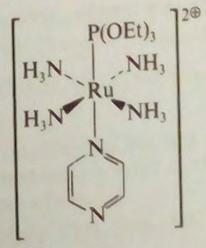
Diperchlorate: [17855-72-0]. *Uranyl perchlorate pentakis(dimethyl sulfoxide)*
$C_{10}H_{30}Cl_2O_{15}S_5U$ M 859.6
Slightly air-sensitive yellow-green cryst. Sol. MeCN, Me_2CO. Approx. pentagonal bipyramidal, 7-coordinate struct. Ir $\nu_{O=U=O}$ 929 cm^{-1} (nujol). Possibly photosensitive.
▷ Explosion hazard.

[55945-24-9]

Nikol'skaya, L.E. *et al*, *CA*, 1975, **83**, 18039 (*ir*)
Vigato, P.A. *et al*, *Gazz. Chim. Ital.*, 1977, **107**, 61 (*synth, ir*)
Honan, G.J. *et al*, *J. Solution Chem.*, 1978, **7**, 443 (*synth, pmr*)
Ikeda, Y. *et al*, *Bull. Res. Lab. Nucl. React. (Tokyo Inst. Technol.)*, 1979, 47; *CA*, **91**, 113027 (*pmr*)
Harrowfield, J.Mac.B. *et al*, *J. Chem. Soc., Dalton Trans.*, 1983, 393 (*cryst struct*)

$C_{10}H_{31}N_6O_3PRu^{2\oplus}$ IC-007212

Tetraammine(pyrazine-N^1)(triethyl phosphite-*P*) ruthenium(*II*)(2+)



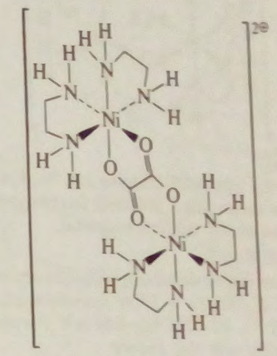
M 415.4 (ion)
Prepd. by treating Tetraammineaqua(triethyl phosphite-*P*) ruthenium(*II*)(2+), IC-005552 with an excess of pyrazine. Sol. H_2O.

Bis-hexafluorophosphate: [64939-10-2].
Orange cryst.

Franco, D.W. *et al*, *Inorg. Chem.*, 1978, **17**, 571 (*synth, uv*)

$C_{10}H_{32}N_8Ni_2O_4^{2\oplus}$ IC-007213

Tetrakis(ethylenediamine-*N,N′*)-μ-oxalatodinickel(*II*) (2+)
μ-Oxalatobis[bis(ethylenediamine)nickel(II)]. *Tetrakis(1,2-ethanediamine*-N,N′)[μ-[ethanedioato(2−)-O,O‴:O′,O″]] *dinickel*(2+), *11CI*

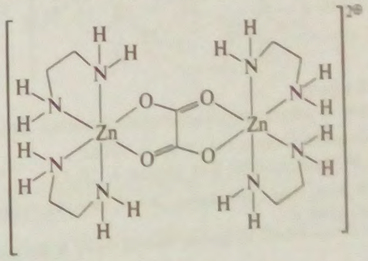


M 445.7 (ion)
Approx. octahedral coordination around Ni.
Dinitrate: [50797-92-7].
Synth. from $Ni(NO_3)_2$, $[Ni(H_2NCH_2CH_2NH_2)_3](ClO_4)_2$ and $Na_2C_2O_4$. Blue-violet cryst. (hot H_2O). Paramagnetic.
Perchlorate: [52675-37-3].
Blue-violet cryst. (hot H_2O). Paramagnetic, μ_{eff} = $3.00\mu_B$ (288K). Potentially explosive.

Curtis, N.F., *J. Chem. Soc.*, 1963, 4109 (*synth, props, ir, deriv*)
Curtis, N.F., *J. Chem. Soc. A*, 1968, 1584 (*uv, perchlorate*)
Curtis, N.F. *et al*, *J. Chem. Soc., Dalton Trans.*, 1973, 1537 (*cryst struct, nitrate*)

$C_{10}H_{32}N_8O_4Zn_2^{2\oplus}$ IC-007214

Tetrakis(ethylenediamine)(μ-oxalato)dizinc(2+)
Tetrakis(1,2-ethanediamine-N,N′)[μ-[*ethanedioato*(2−)-O,O‴:O′,O″]]*dizinc*(2+)

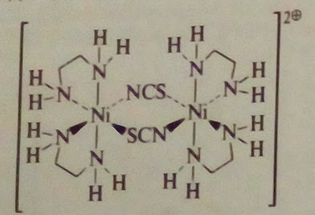


M 459.1 (ion)
Diiodide: [64926-68-7].
Cryst.
Dinitrate: [52691-51-7].
Cryst.
Diperchlorate: [21268-17-7].
Cryst. (H_2O).
▷ Potentially explosive.
Dithiocyanate: [52691-50-6].
Cryst.

Curtis, N.F., *J. Chem. Soc. A*, 1968, 1584 (*synth, ir, perchlorate*)
Skvelashvili, A.E., *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 307 (*synth, struct*)
Burshtein, I.F. *et al*, *Kristallokhim. Neorg. Soedin.*, 1976, 163; *CA*, 1978, **88**, 30594 (*synth, cryst struct, iodide*)

$C_{10}H_{32}N_{10}Ni_2S_2^{2\oplus}$ IC-007215

Tetrakis(1,2-ethanediamine)bis[μ-(thiocyanato-*N*:*S*)]dinickel(*II*)(2+), 9CI



M 473.9 (ion)

Dimeric struct. with NCS bridging oct. Ni. Conflicting reports on magnetism - probably ferromagnetic but also reported as weakly antiferromagnetic.

Diiodide: [20658-31-5].

Synth. from Bis(ethylenediamine)bis(thiocyanato-*N*)nickel(*II*), IC-005283 + $I^{\ominus}$ or Bis(ethylenediamine)nickel(*II*)(2+), IC-004376 iodide salt. Purple solid. Dec. at 250°. Other salts also known.

Babalva, A.V. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1960, **5**, 1055 (*synth*)

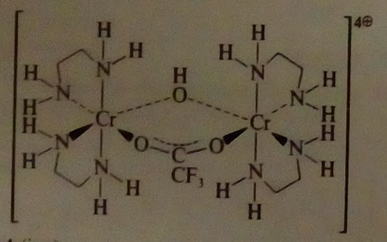
Svelasvili, A.E., *Acta Crystallogr., Sect. A*, 1966, **21**, 153 (*cryst struct*)

Ginsberg, A.P. *et al*, *Inorg. Chem.*, 1972, **11**, 2884 (*synth, magnetism*)

Bogdanov, A.P. *et al*, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1982, **27**, 1455 (*w, magnetism*)

$C_{10}H_{33}Cr_2F_3N_8O_3^{4\oplus}$ IC-007216

Tetrakis(ethylenediamine-*N*,*N*′)-μ-hydroxy-μ-(trifluoroacetato-*O*,*O*′)dichromium(*III*)(4+)



M 474.4 (ion)

Example of μ-hydroxo-μ-carboxylato dinuclear cation.

Tetrabromide: Orange red cryst. + $4H_2O$.

Bromide, triperchlorate: Red prisms + $1H_2O$.

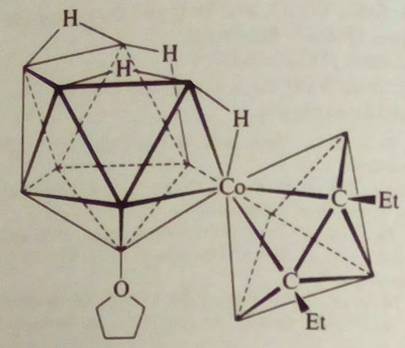
Kaas, K. *et al*, *Acta Chem. Scand., Ser. A*, 1986, **40**, 515 (*cryst struct, synth, vis*)

Compr. Coord. Chem., Pergamon, Oxford, 1987, **3**, 800 (*rev*)

$C_{10}H_{34}B_{13}CoO$ IC-007217

[(2,3,4,5,6-η)-2,3-Diethyl-1,4,5,6-tetrahydro-2,3-dicarbahexaborato(1−)][η⁴-dodecahydro(tetrahydrofuran)nonaborato(2−)-*H*]cobalt, 11CI

[80583-52-4]



M 369.8

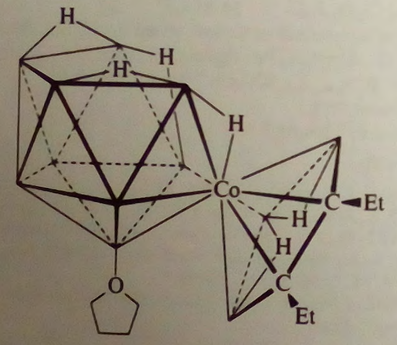
Air-stable brown cryst. (CH_2Cl_2/hexane by chromatog.). Sol. $CHCl_3$, CH_2Cl_2. Mp 89-91°.

Borodinsky, L. *et al*, *Inorg. Chem.*, 1982, **21**, 1921, 1928 (*synth, ir, pmr, ms, B-11 nmr, cryst struct*)

$C_{10}H_{35}B_{12}CoO$ IC-007218

[η⁵-1,2-(1,2-Diethyl-1,2-ethenediyl)triborane(7)][η⁴-dodecahydro(tetrahydrofuran)nonaborato(2−)-*H*]cobalt, 11CI

[80593-35-7]



M 360.0

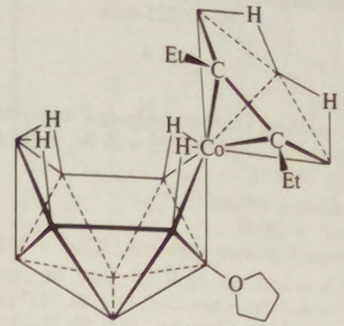
Air-stable orange cryst. (CH_2Cl_2/hexane by chromatog.). Sol. $CHCl_3$, CH_2Cl_2. Mp 141-143°.

Borodinsky, L. *et al*, *Inorg. Chem.*, 1982, **21**, 1921, 1928 (*synth, ir, pmr, ms, B-11 nmr, cryst struct*)

$C_{10}H_{35}B_{12}CoO$ IC-007219

[η⁵-1,2-(1,2-Diethyl-1,2-ethenediyl)triborane(7)][η³-dodecahydro(tetrahydrofuran)nonaborato(2−)-*H*,*H*′]cobalt, 11CI

[80643-03-4]



M 360.0

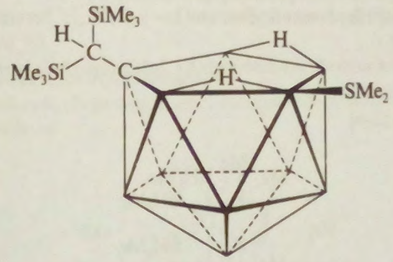
Burgundy cryst. (CH_2Cl_2/hexane by chromatog.). Sol. $CHCl_3$, CH_2Cl_2. Mp 125-127°.

Borodinsky, L. *et al*, *Inorg. Chem.*, 1982, **21**, 1921 (*synth, ir, pmr, B-11 nmr, ms, struct*)

$C_{10}H_{36}B_{10}SSi_2$ IC-007220

7-[Bis(trimethylsilyl)methyl]-9-(dimethyl sulfide)-7-carbaundecaborane(12)

[105335-10-2]



M 352.7

nido-. Positions of bridging H's tentative. Monocarbon carbaborane formed from Decaborane(14), IC-001235. White solid (CH_2Cl_2). Sol. CH_2Cl_2. Mp 147-148°.

Ernest, R.L. *et al*, *Organometallics*, 1987, **6**, 80 (*synth, B-11 nmr, pmr, ir, ms*)

$C_{10}H_{36}Cl_3O_{13}Y$ IC-007221

Trichloro(15-crown-5)yttrium(*III*) octahydrate

Yttrium(III) *chloride 15-crown-5 octahydrate*

$[Y(OH_2)_8]Cl_3$(15-crown-5)

M 559.6

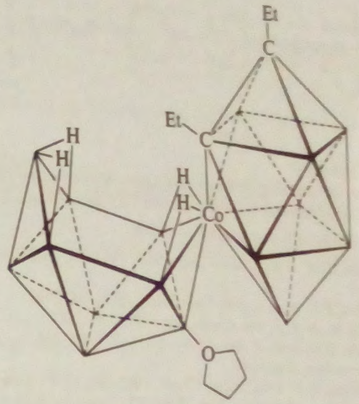
Colourless cryst. (MeOH/MeCN). Mp 104-108°. H_2O hydrogens are hydrogen-bonded to chlorides and oxygens in crown ethers.

Rogers, R.D. *et al*, *Inorg. Chim. Acta*, 1986, **116**, 171 (*synth, cryst struct, ir*)

$C_{10}H_{37}B_{16}CoO$ IC-007222

[η⁵-*C*,*C*′-Diethylheptahydrodicarbanonaborato(1−)][η³-dodecahydro(tetrahydrofuran)nonaborato(1−)-*H*,*H*′]cobalt, 11CI

[80612-07-3]



M 405.3

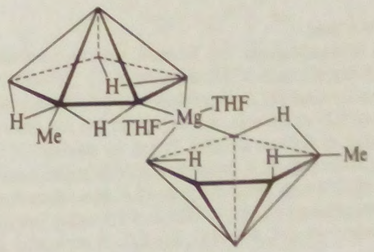
Black-brown cryst. (CH_2Cl_2/hexane by chromatog.). Sol. $CHCl_3$, CH_2Cl_2. Mp 150° dec.

Borodinsky, L. *et al*, *Inorg. Chem.*, 1982, **21**, 1921, 1928 (*synth, ir, pmr, B-11 nmr, ms, cryst struct*)

$C_{10}H_{38}B_{12}MgO_2$ IC-007223

Bis[2-methyloctahydrohexaborato(1−)]magnesium complex with THF (1:2)

[76466-43-8]



M 344.4

nido-. Fluxional in soln. Synth. from $MgMe_2$ in THF and 2-MeB_6H_9 at −78°. White solid. Sol. CH_2Cl_2, $CHCl_3$.

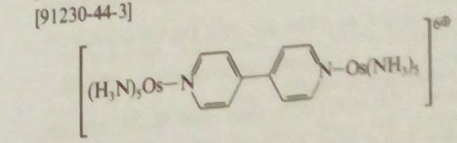
Shore, S.G., *Inorg. Chem.*, 1976, **15**, 541; 1981, **20**, 1270 (*synth, pmr, B-11 nmr*)

$C_{10}H_{38}N_{12}Os_2^{6\oplus}$ IC-007224

Decaammine[μ-(4,4′-bipyridine-*N*,*N*′)]diosmium(*III*)(6+), 11CI

μ-(4,4′-Bipyridine)bis[pentaammineosmium(III)](6+)

[91230-44-3]



M 706.8 (ion)

No salts isol.

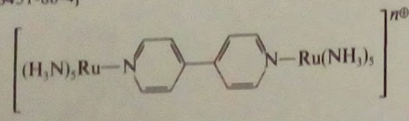
Dubicki, L. *et al*, *J. Phys. Chem.*, 1984, **88**, 3940 (*uv, mcd*)

$C_{10}H_{38}N_{12}Ru_2^{4\oplus}$ IC-007225

Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(4+), 9Cl

μ-4,4′-Bipyridine-bis[pentaammineruthenium(II)]

[36451-88-4]



$n = 4$

M 528.6 (ion)

Prepd. by treating Pentaammine(aqua)ruthenium(*II*)(2+), IC-019980 with 4,4′-bipy in Me_2CO. Sol. Me_2CO, H_2O.

Tetrakis-hexafluorophosphate: Solid.

Lavallee, D.K. *et al, J. Am. Chem. Soc.*, 1972, **94**, 2583 (*synth, uv, pmr*)
Fleischer, E.B. *et al, J. Am. Chem. Soc.*, 1972, **94**, 2599.
Tom, G.M. *et al, J. Am. Chem. Soc.*, 1974, **96**, 7827.
Lavallee, D.K. *et al, J. Am. Chem. Soc.*, 1977, **99**, 718 (*electrochem. oxidation*)
Richardson, D.E. *et al, Inorg. Chem.*, 1981, **20**, 1278 (*electrochem*)
Moore, K.J. *et al, Inorg. Chem.*, 1983, **22**, 1108 (*electrochem*)
Doorn, S.K. *et al, J. Am. Chem. Soc.*, 1990, **112**, 4999 (*raman*)

$C_{10}H_{38}N_{12}Ru_2^{5\oplus}$ IC-007226

Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(5+), 9Cl

μ-4,4′-Bipyridine-bis[pentaammineruthenium(III,II)]

[54065-65-5]

As Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(4+), IC-007225 with

$n = 5$

M 528.6 (ion)

Class II mixed-valence ion. In equil. with Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(6+), IC-007227 and Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(4+), IC-007225 in aq. soln. An important ion for theoretical studies of electron transfer. Prepd. by mixing Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(6+), IC-007227 with Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)] diruthenium(4+), IC-007225 in a 1:1 ratio. Only prepd. in soln.; not isol. Sol. H_2O, Me_2CO. A molecular switch.

Tom, G.M. *et al, J. Am. Chem. Soc.*, 1974, **96**, 7827 (*synth, electrochem, uv, ir*)
Fischer, H. *et al, J. Am. Chem. Soc.*, 1976, **98**, 5512 (*electron transfer reaction*)
Cannon, R.D., *Chem. Phys. Lett.*, 1977, **49**, 299 (*classification*)
Taube, H. *et al, Ann. N.Y. Acad. Sci.*, 1978, **313**, 481 (*electron transfer*)
Creutz, C., *Inorg. Chem.*, 1978, **17**, 3723 (*optical electron transfer*)
Sutton, J.E. *et al, Inorg. Chem.*, 1979, **18**, 1017 (*electrochem, uv, ir*)
Richardson, D.E. *et al, Inorg. Chem.*, 1981, **20**, 1278 (*electrochem*)
Sutton, J.E. *et al, Inorg. Chem.*, 1981, **20**, 3125 (*analogues*)
Moore, K.J. *et al, Inorg. Chem.*, 1983, **22**, 1108 (*electrochem*)
Hupp, J.T. *et al, Inorg. Chem.*, 1987, **26**, 2332, 2657 (*electron transfer*)
Isied, S.S. *et al, J. Am. Chem. Soc.*, 1988, **110**, 635 (*electron transfer*)
Launay, J.P. *et al, J. Chim. Phys. Phys.-Chim. Biol.*, 1988, **85**, 1135 (*use, electron transfer*)
Blackbourn, R.L. *et al, J. Phys. Chem.*, 1988, **92**, 2817 (*electron transfer*)
Woitellier, S. *et al, Chem. Phys.*, 1989, **131**, 481 (*use, theory*)
Reimers, J.R. *et al, Inorg. Chem.*, 1990, **29**, 3686 (*electron transfer, uv, theory*)
Doorn, S.K. *et al, J. Am. Chem. Soc.*, 1990, **112**, 4999 (*raman*)

$C_{10}H_{38}N_{12}Ru_2^{6\oplus}$ IC-007227

Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(6+), 9Cl

μ-4,4′-Bipyridinebis[pentaammineruthenium(III)]

[53964-47-9]

As Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)]diruthenium(4+), IC-007225 with

$n = 6$

M 528.6 (ion)

Prepd. by oxidising Decaammine[μ-(4,4′-bipyridine-*N*:*N*′)] diruthenium(4+), IC-007225 with Br_2 in 0.1*M* HCl. Sol. H_2O, Me_2CO.

Hexa-perchlorate: [69042-75-7].
Red cryst. + $2H_2O$.

Hexakis-(4-methylbenzenesulfonate): Solid + $1H_2O$.

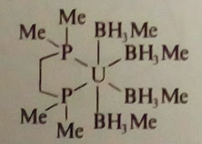
Fleischer, E.B. *et al, J. Am. Chem. Soc.*, 1972, **94**, 2599 (*synth*)
Tom, G.M. *et al, J. Am. Chem. Soc.*, 1974, **96**, 7827 (*synth*)
Fischer, H. *et al, J. Am. Chem. Soc.*, 1976, **98**, 5512 (*electron-transfer reactions*)
Sutton, J.E. *et al, Inorg. Chem.*, 1979, **18**, 1017 (*synth, uv, ir, electrochem*)
Moore, K.J. *et al, Inorg. Chem.*, 1983, **22**, 1108 (*electrochem*)
Hupp, J.T. *et al, Inorg. Chem.*, 1987, **26**, 2657 (*electron transfer, uv*)
Reimers, J.R. *et al, Inorg. Chem.*, 1990, **29**, 3686 (*electron transfer, uv, theory*)
Doorn, S.K. *et al, J. Am. Chem. Soc.*, 1990, **112**, 4999 (*raman*)

$C_{10}H_{40}B_4P_2U$ IC-007228

[1,2-Ethanediylbis[dimethylphosphine]-*P*,*P*′] tetrakis[trihydromethylborato(1−)-*H*,*H*′,*H*″]uranium, 11Cl

Tetrakis(methyltrihydroborato)[1,2-bis(dimethylphosphino) ethane]uranium

[92958-52-6]



M 503.6

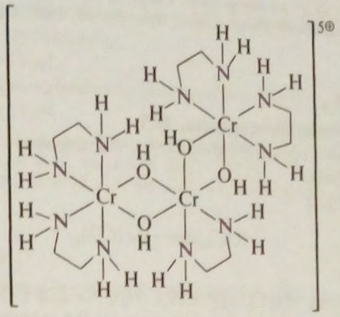
On heating at 80° in toluene with 1,2-bis(dimethylphosphino)ethane affords Bis[1,2-ethanediylbis[dimethylphosphine]-*P*,*P*′] tris[trihydromethylborato(1−)-*H*,*H*′,*H*″]uranium, IC-009180. Air- and moisture-sensitive green cryst. Sol. toluene. Mp 131-132° dec.

Brennan, J. *et al, Inorg. Chem.*, 1984, **23**, 4143 (*synth, cryst struct, nmr*)

$C_{10}H_{44}Cr_3N_{10}O_4^{5\oplus}$ IC-007229

μ-[(Ethylenediamine)tetrahydroxochromium(*III*)] bis[bis(ethylenediamine)chromium(*III*)](5+)

*Pentakis(1,2-ethanediamine-*N,N′*)tetra-μ-hydroxytrichromium*(III)(5+)



M 524.5 (ion)

Structural assignment based only on analyses and hydrol. products. Hydrol. (70% $HClO_4$) gives *cis*-$[Cr(H_2O)_2(en)_2]^{3\oplus}$ and $[Cr(H_2O)_4(en)]^{3\oplus}$ (2:1).

Pentaiodide: [69786-51-2].
Obt. by ion exchange sepn. of aq. $[Cr(en)_3]Cl_3$,$[enH_2]Cl_2$ and enafter 3-5 days at 40-50°.

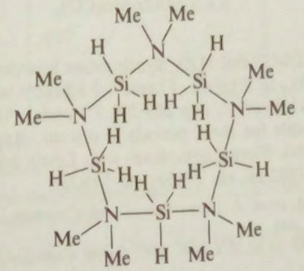
Pentanitrate: [69786-50-1].
Synth. from crude iodide in 70% EtOH + $LiNO_3$. Violet cryst. (70% aq. EtOH, $LiNO_3$).

Andersen, P. *et al, Acta Chem. Scand., Ser. A*, 1978, **32**, 989 (*synth*)

$C_{10}H_{45}N_5Si_5$ IC-007230

Pentakis(dimethylaminosilane)

Pentadecahydropentakis[μ-(N-methylmethaniminato)] pentasilicon



M 375.9

First crystallographically verified example of penta-coordinated Si. Synth. from $NHMe_2$ and SiH_3Br. Colourless cryst. Mp 3.3-3.4°.

Sujishi, S. *et al, J. Am. Chem. Soc.*, 1954, **76**, 4631 (*synth*)
Rudman, R. *et al, J. Am. Chem. Soc.*, 1967, **89**, 5157 (*cryst struct*)
Blake, A.J. *et al, Acta Crystallogr., Sect. C*, 1984, **40**, 895 (*cryst struct*)

$C_{10}HgMn_2O_{10}$ IC-007231

Bis(pentacarbonylmanganese)mercury

Decacarbonyl(mercury)dimanganese, 9Cl. Decacarbonyl-μ-mercuriodimanganese, 8Cl. Decacarbonyldimanganesemercury

[15525-07-2]

$(OC)_5MnHgMn(CO)_5$

M 590.5

Synth. from $HgSO_4$ or $Hg(CN)_2$ and $Na[Mn(CO)_5]$. Pale-yellow cryst. (toluene). $Subl._{0.1}$ 100-140°. Dec. at 155°. Forms THF complex. Ir ν_{CO} 2059, 2006, 1969 cm^{-1} (solid).

Hieber, W. *et al, Chem. Ber.*, 1960, **93**, 455 (*synth, ir*)
King, R.B., *J. Inorg. Nucl. Chem.*, 1963, **25**, 1296.
Brier, P.N. *et al, J. Chem. Soc. A*, 1967, 1889 (*ir*)
Adams, D.M. *et al, J. Chem. Soc. A*, 1968, 2817 (*ir, raman*)
King, R.B., *Org. Mass Spectrom.*, 1969, **2**, 657 (*ms*)
Hsieh, A.T.T. *et al, J. Chem. Soc. A*, 1971, 729 (*ir, raman*)
Katcher, M.L. *et al, Inorg. Chem.*, 1972, **11**, 1651 (*ir, ms, cryst struct*)
Kinstle, G.P. *et al, Inorg. Chim. Acta*, 1979, **32**, L61 (*deriv, ir*)

$C_{10}I_2O_{10}Os_3$ IC-007232

Decacarbonyldi-μ-iodotriosmium, 8Cl

[28109-20-8]

As Di-μ-bromodecacarbonyltriosmium, IC-006659 with

X = I

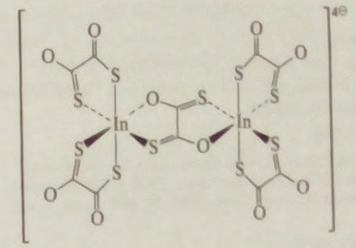
M 1104.5

Orange cryst. (pentane).

Deeming, A.J. *et al, J. Chem. Soc. A*, 1970, 897 (*synth, ir*)
Bryan, E.G. *et al, J. Chem. Soc., Chem. Commun.*, 1977, 329 (*cmr*)
Vaglio, G.A., *J. Organomet. Chem.*, 1979, **169**, 83 (*ms*)

$C_{10}In_2O_{10}S_{10}^{4\ominus}$ IC-007233

1,2-(μ-*trans*-Dithiooxalato)tetrakis(dithiooxalato-*S*,*S*′) diindate(4−)



M 830.4 (ion)

Tetrakis-Ph_4As salt: [79725-63-6].
Synth. from In and $K_2C_2S_2O_2$ in aq. EtOH, and Ph_4AsCl in CH_2Cl_2. Yellow cryst. ($MeNO_2$/Et_2O).

Dietzsch, W. *et al, Z. Chem.*, 1981, **21**, 269 (*synth*)
Golič, L. *et al, Inorg. Chem.*, 1982, **21**, 3560 (*synth, cryst struct*)

$C_{10}MnMoO_{10}^{\ominus}$ IC-007234

Pentacarbonyl(pentacarbonylmanganate)molybdate(1−), 11Cl

Decacarbonylmolybdatemanganate(1−). Pentacarbonyl(pentacarbonylmolybdenio)manganate(1−)

$[(OC)_5Mn{-}Mo(CO)_5]^{\ominus}$

M 430.9 (ion)

Synth. from $Na[Mn(CO)_5]$ and $Mo(CO)_6$ in diglyme.

Et_4N salt: [19663-43-5].
Yellow cryst. (EtOH aq.). Ir ν_{CO} 2067w, 2007s, 1946vs, 1920m, 1904w, 1866s cm^{-1} (THF).

Anders, U. *et al, J. Am. Chem. Soc.*, 1967, **89**, 539 (*synth, ir*)
Ruff, J.K., *Inorg. Chem.*, 1968, **7**, 1818 (*synth*)
Onaka, S. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 257 (*O-17 nmr*)

$C_{10}MnO_{10}Re$ IC-007235

Pentacarbonyl(pentacarbonylmanganese)rhenium, 8CI

Manganese rhenium decacarbonyl.
Decacarbonylmanganeserhenium

[14693-30-2]

$(OC)_5Re—Mn(CO)_5$

M 521.2
Synth. from $NaMn(CO)_5$ and $ReBr(CO)_5$ or by photolysis of $Mn_2(CO)_{10}$ and $Re_2(CO)_{10}$. White, air-stable cryst. purif. by gc. Products obt. from $MnBr(CO)_5$ and $NaRe(CO)_5$ are mainly mixt. of $Mn_2(CO)_{10}$ and $Re_2(CO)_{10}$.

Nesmeyanov, A.N. *et al, Izv. Akad. Sci. USSR, Ser. Sci. Khim.*, 1963, 194 (*synth*)
Struchkov, Y.T. *et al, Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1967, **172**, 107 (*cryst struct*)
Evans, G.O. *et al, J. Inorg. Nucl. Chem.*, 1968, **30**, 2862 (*synth*)
Junk, G.A. *et al, J. Chem. Soc. A*, 1970, 2102 (*ms*)
Spiro, T.G., *Prog. Inorg. Chem.*, 1970, **11**, 1 (*raman*)
Knox, S.A.R. *et al, Inorg. Chem.*, 1971, **10**, 2636 (*synth, ir, raman*)
Abel, E.W. *et al, Inorg. Nucl. Chem. Lett.*, 1971, **7**, 587 (*synth*)
Jackson, R.A. *et al, Inorg. Chem.*, 1978, **17**, 997 (*uv*)
Michels, G.D. *et al, Inorg. Chem.*, 1981, **20**, 3445 (*synth, ir, ms*)

$C_{10}MnO_{10}Tc$ IC-007236

Pentacarbonyl(pentacarbonylmanganese)technetium, 10CI

[71619-58-4]

$(OC)_5Mn—Tc(CO)_5$

M 433.9
Synth. from $TcBr(CO)_5$ + $[Mn(CO)_5]^{\ominus}$ or from $^{99}Tc^{m}(CO)_5$ radicals from β-decay of $^{99}Mo(CO)_5$ and $Mn(CO)_5$ radicals.

[41375-72-8]

De Jong, I.G. *et al, Inorg. Chem.*, 1973, **12**, 2519 (*synth*)
Michels, G.D., *Energy Res. Abstr.*, 1979, **4**, 30986 (*synth*)
Michels, G.D., *Inorg. Chem.*, 1981, **20**, 3445 (*synth, ir, ms*)

$C_{10}MnO_{10}W^{\ominus}$ IC-007237

Pentacarbonyl(pentacarbonylmanganate)tungstate(1 –), 11CI

Decacarbonyltungstatemanganate(1 –).
Pentacarbonyl(pentacarbonyltungstenio)manganate(1 –)

$[(OC)_5Mn—W(CO)_5]^{\ominus}$

M 518.8 (ion)
Synth. from $NaMn(CO)_5$ + $W(CO)_6$ in diglyme.
Et_4N salt: [19663-44-6].
Yellow cryst. (EtOH aq.). Ir ν_{CO} 2066w, 2007s, 1948vs, 1926m, 1898s, 1861m cm^{-1} (THF).

Anders, U. *et al, J. Am. Chem. Soc.*, 1967, **89**, 539 (*synth, ir*)
Ruff, J.K., *Inorg. Chem.*, 1968, **7**, 1818 (*synth*)
Onaka, S. *et al, J. Chem. Soc., Dalton Trans.*, 1982, 257 (*O-17 nmr*)

$C_{10}Mn_2N_{10}O^{6\ominus}$ IC-007238

Decakis(cyano-*C*)-μ-oxodimanganate(6 –), 11CI

μ-Oxobis[pentacyanomanganate(III)]

[54204-64-7]

$[(NC)_5Mn\text{-}O\text{-}Mn(CN)_5]^{6\ominus}$

M 386.0 (ion)
Bioctahedral anion with eclipsed rotomeric config.
Hexa-K salt: [54204-65-8].
Synth. from $KMnO_4$ + KCN. Golden brown pleochroic cryst. + KCN, stable in dry air and light. Insol. polar and non-polar solvs. Diamagnetic at r.t.

Ziolo, R.F. *et al, J. Am. Chem. Soc.*, 1974, **96**, 7910 (*synth, cryst struct, magnetism, uv, ir*)
Trageser, G. *et al, Inorg. Nucl. Chem. Lett.*, 1978, **14**, 65 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1980, **D2**, 241 (*rev, bibl*)

$C_{10}Mn_2O_{10}$ IC-007239

Decacarbonyldimanganese, 8CI

Manganese carbonyl ($Mn_2(CO)_{10}$). Dimanganese decacarbonyl

[10170-69-1]

$(OC)_5Mn—Mn(CO)_5$

M 389.9
Synth. from $Mn(CO)_3(\eta^5\text{-}CH_3C_5H_4)$, Na and CO in refluxing diglyme. Starting material for manganese carbonyl chemistry. Yellow cryst. Sol. org. solvs. Mp 152-154°. $Subl._{0.1}$ 80°.

Podall, H.E. *et al, J. Am. Chem. Soc.*, 1960, **82**, 1325 (*synth*)
Calderazzo, F. *et al, Inorg. Chem.*, 1965, **4**, 293 (*synth*)
Lewis, J. *et al, J. Chem. Soc. A*, 1966, 1663 (*ms*)
Haas, H. *et al, J. Chem. Phys.*, 1967, **47**, 2996 (*ir*)
King, R.B., *J. Organomet. Chem.*, 1968, **11**, 641 (*synth*)
Almenningen, A. *et al, Acta Chem. Scand.*, 1969, **23**, 865 (*cryst struct*)
Brill, T.B. *et al, Inorg. Chem.*, 1974, **13**, 470 (*synth*)
Ireland, P.S. *et al, J. Magn. Reson.*, 1976, **23**, 485 (*nmr*)

$C_{10}Mn_2O_{10}Zn$ IC-007240

Bis(pentacarbonylmanganese)zinc

Decacarbonyl-μ-zinciodimanganese, 8CI. Decacarbonyl(zinc) dimanganese. Decacarbonyldimanganesezinc

[21686-75-9]

$(OC)_5MnZnMn(CO)_5$

M 455.3
Ionises in DMF and H_2O. Synth. from powdered Zn and $Mn_2(CO)_{10}$ in diglyme. Forms 1:2 adducts with nitrogen bases. White cryst. Mp 208-209.5° (under Ar). $Subl._{0.001}$ 120°. Stable for short periods in dry air. Rapid dec. in polar solvs. Forms complexes with Lewis bases. Ir ν_{CO} 2065m, 1985ms, sh, 1945vs cm^{-1} (KBr).

Burlitch, J.M. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 887 (*synth, ir, ms*)
Carey, N.A.D. *et al, J. Chem. Soc., Chem. Commun.*, 1968, 1471 (*synth*)
Hsieh, A.T.T. *et al, J. Chem. Soc. A*, 1971, 729 (*ir, raman, derivs*)
Burlitch, J.M. *et al, Organometallics*, 1982, **1**, 1074 (*synth*)

$C_{10}MoO_{10}Re^{\ominus}$ IC-007241

Pentacarbonyl(pentacarbonylrhenate)molybdate(1 –), 9CI

Decacarbonylmolybdaterhenate(1 –)

$[(OC)_5Re—Mo(CO)_5]^{\ominus}$

M 562.2 (ion)
Et_4N salt: [14874-51-2].
Orange-yellow cryst. (EtOH aq.). Ir ν_{CO} 2073w, 2009s, 1954vs, 1925m, 1901s, 1853m cm^{-1} (THF).

Anders, U. *et al, J. Am. Chem. Soc.*, 1967, **89**, 539 (*synth, ir*)
Johnson, J.R. *et al, Inorg. Chem.*, 1975, **14**, 1053 (*ir, uv, raman*)

$C_{10}Mo_2O_{10}^{2\ominus}$ IC-007242

Decarbonyldimolybdate(2 –), 9CI

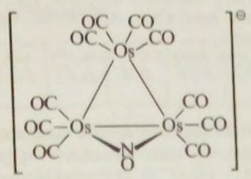
$[(OC)_5Mo—Mo(CO)_5]^{2\ominus}$

M 471.9 (ion)
Staggered conformation. Mo—Mo distance 212.3 pm.
Di-K salt: [57348-62-6].
Yellow cryst.
Bis[bis(triphenylphosphine)iminium] salt: [49736-19-8].
Yellow cryst.

Hayter, R.G., *J. Am. Chem. Soc.*, 1966, **88**, 4376 (*synth*)
Dahl, L.F. *et al, J. Am. Chem. Soc.*, 1970, **92**, 7312 (*cryst struct*)
Ungurenasu, C. *et al, J. Chem. Soc., Chem. Commun.*, 1975, 388 (*synth*)

$C_{10}NO_{11}Os_3^{\ominus}$ IC-007243

Decacarbonyl-μ-nitrosyltriosmate(1 –), 10CI

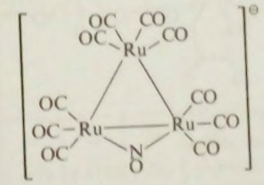


M 880.7 (ion)
Characterised spectroscopically.

Stevens, R.E. *et al, J. Am. Chem. Soc.*, 1981, **103**, 4981 (*synth, ir*)

$C_{10}NO_{11}Ru_3^{\ominus}$ IC-007244

Decacarbonyl-μ-nitrosyltriruthenate(1 –), 10CI



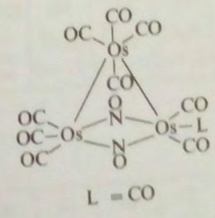
M 613.3 (ion)
Probable struct.
Bis(triphenylphosphine)iminium salt: [79085-63-5].
Green cryst. (Et_2O).

Stevens, R.E. *et al, J. Am. Chem. Soc.*, 1981, **103**, 4981 (*synth, ir*)

$C_{10}N_2O_{12}Os_3$ IC-007245

Decacarbonyldi-μ-nitrosyltriosmium

[36583-25-2]



L = CO

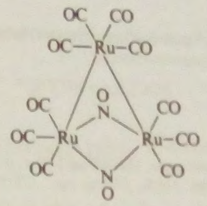
M 910.7
Air-stable light-green cryst. (heptane/C_6H_6).

Norton, J. *et al, Inorg. Chem.*, 1972, **11**, 382 (*synth, ir, ms*)
Inorg. Synth., 1976, **16**, 40 (*synth, ir*)

$C_{10}N_2O_{12}Ru_3$ IC-007246

Decacarbonyldi-μ-nitrosyltriruthenium, 9CI

[36583-24-1]



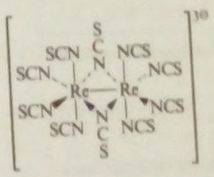
M 643.3
The NO bridges are symmetrical. $Ru—Ru_{unbridged}$ 286.6, $Ru—Ru_{bridged}$ 315.0, N—O 122, Ru—N 203 pm. Synth. from $Ru_3(CO)_{12}$ and NO in boiling C_6H_6 or cyclohexane. Pale green, diamagnetic moderately air-stable cryst. (heptane/pentane). Ir ν_{CO} 2110, 2077, 2068, 2061, 2038, 2030, 2026, 2015, 2000 cm^{-1}, ν_{NO} 1524, 1508 cm^{-1} (hexane).

Norton, J. *et al, J. Am. Chem. Soc.*, 1969, **91**, 7537 (*synth, ir, ms*)
Poliakoff, M. *et al, J. Chem. Soc. A*, 1971, 654 (*ir, matrix isolation*)
Norton, J.R. *et al, Inorg. Chem.*, 1972, **11**, 382 (*synth, cryst struct*)
Forster, A. *et al, J. Chem. Soc., Chem. Commun.*, 1974, 1042 (*cmr*)
Inorg. Synth., 1976, **16**, 39 (*synth, ir*)

$C_{10}N_{10}Re_2S_{10}^{3\ominus}$ IC-007247

Decakis(thiocyanato-*N*)dirhenate(3 –), 10CI

Deca(isothiocyanato)dirhenate(3 –). Bis[μ-(thiocyanato-N,S)]octakis(thiocyanato-N)dirhenate(3 –)



M 953.2 (ion)
Re_2N_{10} core with D_{2h} symmetry and two bridging -NCS groups; mixed valence complex having Re—Re 261.3; Re—N 201.8 to 209.5 pm (Bu_4N salt).
Tris-tetrabutylammonium salt: [71250-44-7].
Obt. from $(Bu_4N)_2Re_2Cl_8$ and NaNCS in Me_2CO. Dark green cryst. ($MeCN/Et_2O$ at –10°).

Cotton, F.A. *et al, Inorg. Chem.*, 1979, **18**, 2719 (*synth, cryst struct, props*)

$C_{10}N_{11}Ru_2^{5\ominus}$ IC-007248

Decakis(cyano-*C*)-μ-nitridodiruthenate(5 –), 9CI

μ-Nitridobis[pentacyanoruthenate(IV)](5 –). Decacyano-μ-nitridodiruthenate(IV)(5 –)

[42735-89-7]

$[(NC)_5Ru{\equiv}N{=}Ru(CN)_5]^{5\ominus}$

M 476.3 (ion)
Hydrolytically inert. Sol. H_2O.
Penta-K salt: [108617-05-6].
Prepd. by treating $[Ru_2NCl_6(OH_2)_2]^{3\ominus}$ with aq. KOH, followed by KCN. Yellow solid + $3H_2O$; diamagnetic. Ir $\nu_{Ru\equiv N}$ 1017, 264 cm^{-1}.

Griffith, W.P. *et al, J. Chem. Soc., Dalton Trans.*, 1973, 1315 (*synth, ir, raman*)

$C_{10}O_{10}ReW^{\ominus}$ – $C_{10}O_{22}V_2^{6\ominus}$

Good, M.L. *et al*, *J. Phys. Chem.*, 1984, **88**, 483.
Griffith, W.P. *et al*, *Inorg. Chim. Acta*, 1987, **126**, 179 (*cryst struct, ir, cmr*)

$C_{10}O_{10}ReW^{\ominus}$ IC-007249

Pentacarbonyl(pentacarbonylrhenate)tungstate(1 –), 9CI
Decacarbonyltungstaterhenate(1 –)

$$[(OC)_5Re—W(CO)_5]^{\ominus}$$

M 650.1 (ion)
Et_4N salt. [19662-36-3].
Orange-yellow cryst. (EtOH aq.). Ir ν_{CO} 2076w, 2009s, 1958vs, 1930m, 1893s, 1857m cm^{-1} (THF).
Anders, U. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 539 (*synth, ir*)
Johnson, J.R. *et al*, *Inorg. Chem.*, 1975, **14**, 1053 (*ir, uv, raman*)

$C_{10}O_{10}Re_2$ IC-007250

Decacarbonyldirhenium, 10CI
Dirhenium decacarbonyl
[14285-68-8]

$$(OC)_5Re—Re(CO)_5$$

M 652.5
White air-stable cryst. by subl. Spar. sol. org. solvs.; insol. H_2O. Mp 177°.
Organomet. Synth., 1965, **1**, 92 (*synth*)
Quicksall, C.O. *et al*, *Inorg. Chem.*, 1969, **8**, 2363 (*ir, raman*)
Swenson, B.I. *et al*, *Prog. Inorg. Chem.*, 1970, **11**, 1 (*ir*)
Bor, G. *et al*, *J. Chem. Soc., Dalton Trans.*, 1974, 440 (*ir, raman*)
Jackson, R.A. *et al*, *Inorg. Chem.*, 1978, **17**, 997 (*uv*)
Churchill, M.R. *et al*, *Inorg. Chem.*, 1981, **20**, 1609 (*cryst struct*)
Calderazzo, F. *et al*, *Gazz. Chim. Ital.*, 1985, **115**, 537 (*synth*)

$C_{10}O_{10}SW_2^{2\ominus}$ IC-007251

Decacarbonyl-μ-thioxoditungstate(2 –), 11CI
[83477-60-5]

$$[(OC)_5W—S—W(CO)_5]^{2\ominus}$$

M 679.8 (ion)
Reacts with organic electrophiles.
Di-Na salt: Yellow needles ($CHCl_3$). Mp 110-113°.
Gingerich, R.G.W. *et al*, *J. Am. Chem. Soc.*, 1978, **101**, 5604 (*uv, synth, ir, nmr*)
Angelici, R. *et al*, *Organometallics*, 1983, **2**, 89 (*props*)

$C_{10}O_{10}Tc_2$ IC-007252

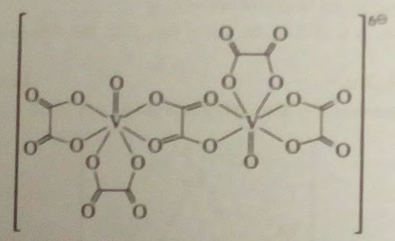
Decacarbonylditechnetium, 10CI
Ditechnetium decacarbonyl. Technetium carbonyl
[14837-15-1]

$$(OC)_5Tc—Tc(CO)_5$$

M 477.9
Diamagnetic. Colourless cryst. (pentane); solns. dec. slowly in air. Mp 159-160°.
[78498-97-2]
Hileman, J.C. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 2953 (*synth, ir, props*)
Hileman, J.C., *Prep. Inorg. React.*, Jolly, W.J., Ed., Interscience, New York, 1964, **1**, 102 (*synth*)
Bailey, M.F. *et al*, *Inorg. Chem.*, 1965, **4**, 1140 (*cryst struct*)
Junk, G.A. *et al*, *J. Chem. Soc. A*, 1970, 2102 (*ms*)
Spiro, T.G., *Prog. Inorg. Chem.*, 1970, **11**, 1 (*ir, raman*)
Jackson, R.A. *et al*, *Inorg. Chem.*, 1978, **17**, 997
Kidd, D.R. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 4095 (*props*)
Gmelin Handbook Inorg. Chem., Syst. No. 69, Suppl. Vol. 2, 1983, 128 (*bibl, rev*)
Findeisen, M. *et al*, *Inorg. Chim. Acta*, 1987, **128**, L15 (*Tc-99 nmr*)

$C_{10}O_{22}V_2^{6\ominus}$ IC-007253

μ-Oxalatotetrakis(oxalato)dioxodivanadate(*IV*)(6 –)
μ-Oxalatobis[oxobis(oxalato)vanadate(IV)]. [μ-[Ethanedioato(2 –)-O,O'':O',O''']]tetrakis[ethanedioato(2 –)-O,O']dioxodivanadate(IV)(6 –), 10CI



M 573.9 (ion)
Tentative struct. shown.
Hexaamminecobalt(3+) salt: [78278-81-6].
Synth. by mixing aq. solns. of $VO(C_2O_4)$ and $[Co(NH_3)_6]_2(C_2O_4)_3$. Yellow solid. Insol. H_2O, org. solvs. Paramagnetic, μ_{eff} = 1.25μ_B (298K).
Bhaumik, B.B. *et al*, *Indian J. Chem., Sect. A*, 1981, **20**, 417 (*synth, ir, tga, dta, magnetism*)

Periodic Table of the Elements

IUPAC Notation

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

Previous IUPAC Notation

IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA	IB	IIB	IIIB	IVB	VB	VIB	VIIB	0

1 H 1.01																	2 He 4.00
3 Li 6.94	4 Be 9.01											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98.91)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57–71 See Lantha-nides	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209.98)	85 At (209.99)	86 Rn (222.02)
87 Fr (223.02)	88 Ra (226.03)	89–103 See Acti-nides	104 Unq (261.11)	105 Unp (262.11)	106 Unh (263.12)	107 Uns (262.12)	108 Uno	109 Une	110 Uun								

57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (144.91)	62 Sm 150.36	63 Eu 151.97	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
89 Ac 227.03	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu (239.05)	95 Am (241.06)	96 Cm (244.06)	97 Bk (249.08)	98 Cf (252.08)	99 Es (252.08)	100 Fm (257.10)	101 Md (256.09)	102 No (259.10)	103 Lr (262.11)

Lanthanides

Actinides